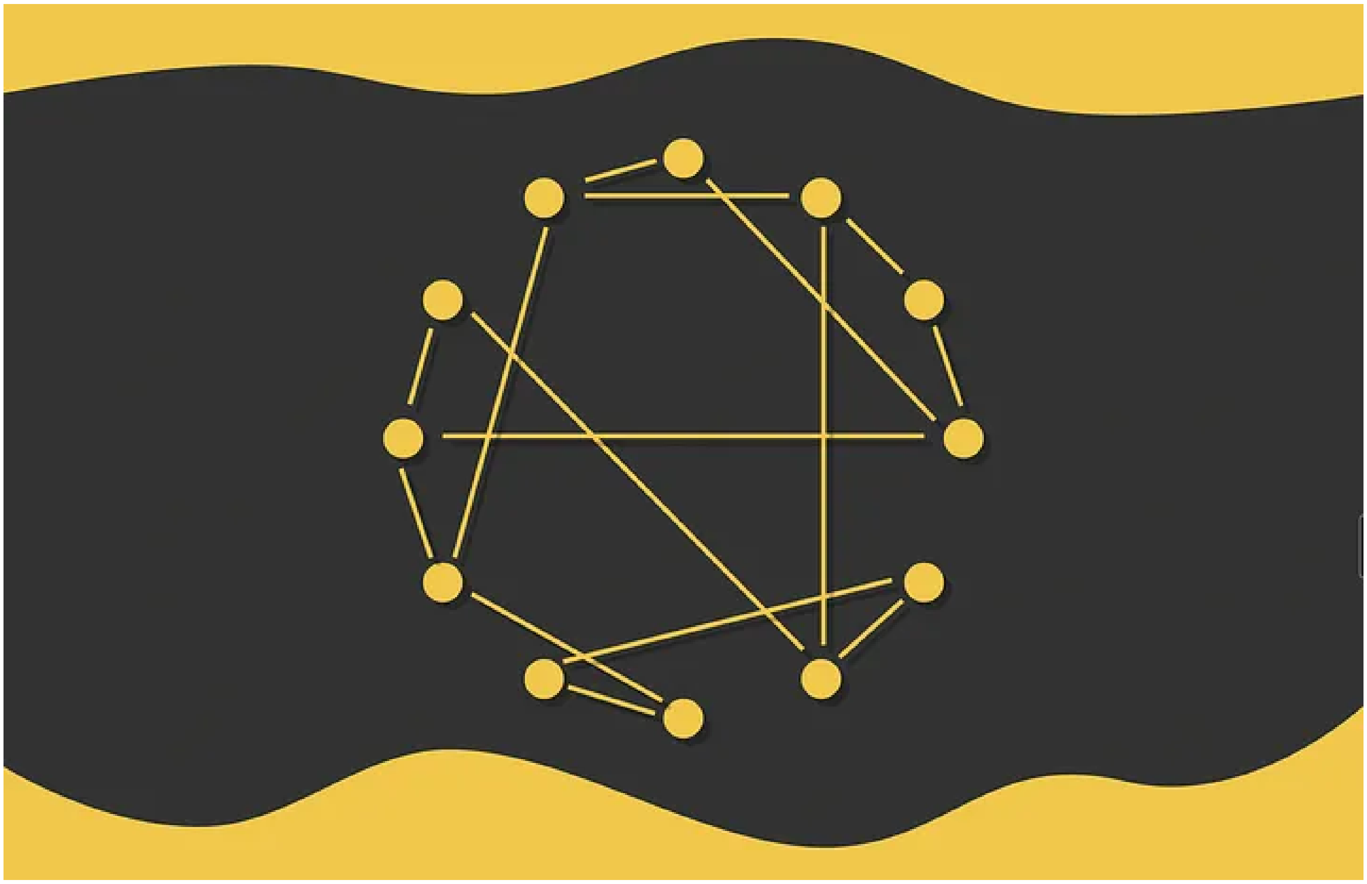
Similarity Search, Part 4: Hierarchical Navigable Small World (HNSW)

Discover how to construct efficient multi-layered graphs to boost search speed in massive volumes of data

Vyacheslav Efimov · Following

Published in Towards Data Science · 13 min read · Jun 16

238 2



Similarity search is a problem where given a query the goal is to find the most similar documents to it among all the database documents.

Introduction

In data science, similarity search often appears in the NLP domain, search engines or recommender systems where the most relevant documents or items need to be retrieved for a query. There exists a large variety of different ways to improve search performance in massive volumes of data.

Hierarchical Navigable Small World (HNSW) is a state-of-the-art algorithm used for an approximate search of nearest neighbours. Under the hood, HNSW constructs optimized graph structures making it very different from other approaches that were discussed in previous parts of this article series.

The main idea of HNSW is to construct such a graph where a path between any pair of vertices could be traversed in a small number of steps.

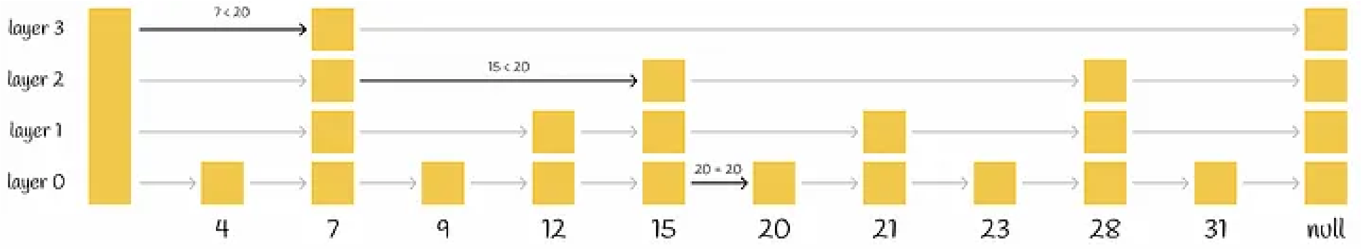
A well-known analogy on the famous six handshakes rule is related to this method:

> *All people are six or fewer social connections away from each other.*

Before proceeding to inner workings of HNSW let us first discuss skip lists and navigable small words — crucial data structures used inside the HNSW implementation.

Skip lists

Skip list is a probabilistic data structure that allows inserting and searching elements within a sorted list for *O(logn)* on average. A skip list is constructed by several layers of linked lists. The lowest layer has the original linked list with all the elements in it. When moving to higher levels, the number of skipped elements increases, thus decreasing the number of connections.



Finding element 20 in skip list

The search procedure for a certain value starts from the highest level and compares its next element with the value. If the value is less or equal to the element, then the algorithm proceeds to its next element. Otherwise, the search procedure descends to the lower layer with more connections and repeats the same process. At the end, the algorithm descends to the lowest layer and finds the desired node.

Based on the information from Wikipedia, a skip list has the main parameter *p* which defines the probability of an element appearing in several lists. If an element appears in layer *i*, then the probability that it will appear in layer *i + 1* is equal to *p (p* is usually set to 0.5 or 0.25*)*. On average, each element is presented in *1 / (1 — p)* lists.

As we can see, this process is much faster than the normal linear search in the linked list. In fact, HNSW inherits the same idea but instead of linked lists, it uses graphs.

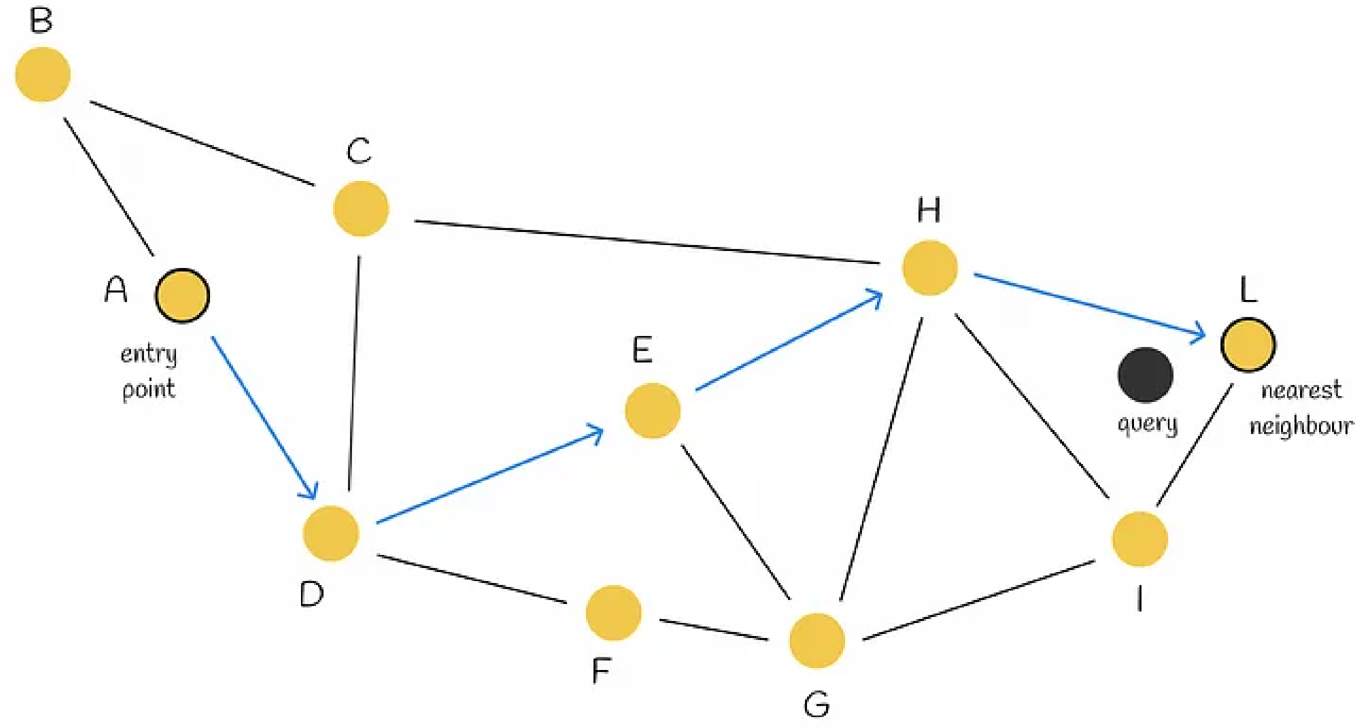
Navigable Small World

Navigable small world is a graph with polylogarithmic $T = O(\log^k n)$ search complexity which uses greedy routing. **Routing** refers to the process of starting the search process from low-degree vertices and ending with high-degree vertices. Since low-degree vertices have very few connections, the algorithm can rapidly move between them to efficiently navigate to the region where the nearest neighbour is likely to be located. Then the algorithm gradually zooms in and switches to high-degree vertices to find the nearest neighbour among the vertices in that region.

> *Vertex is sometimes also referred to as a **node**.*

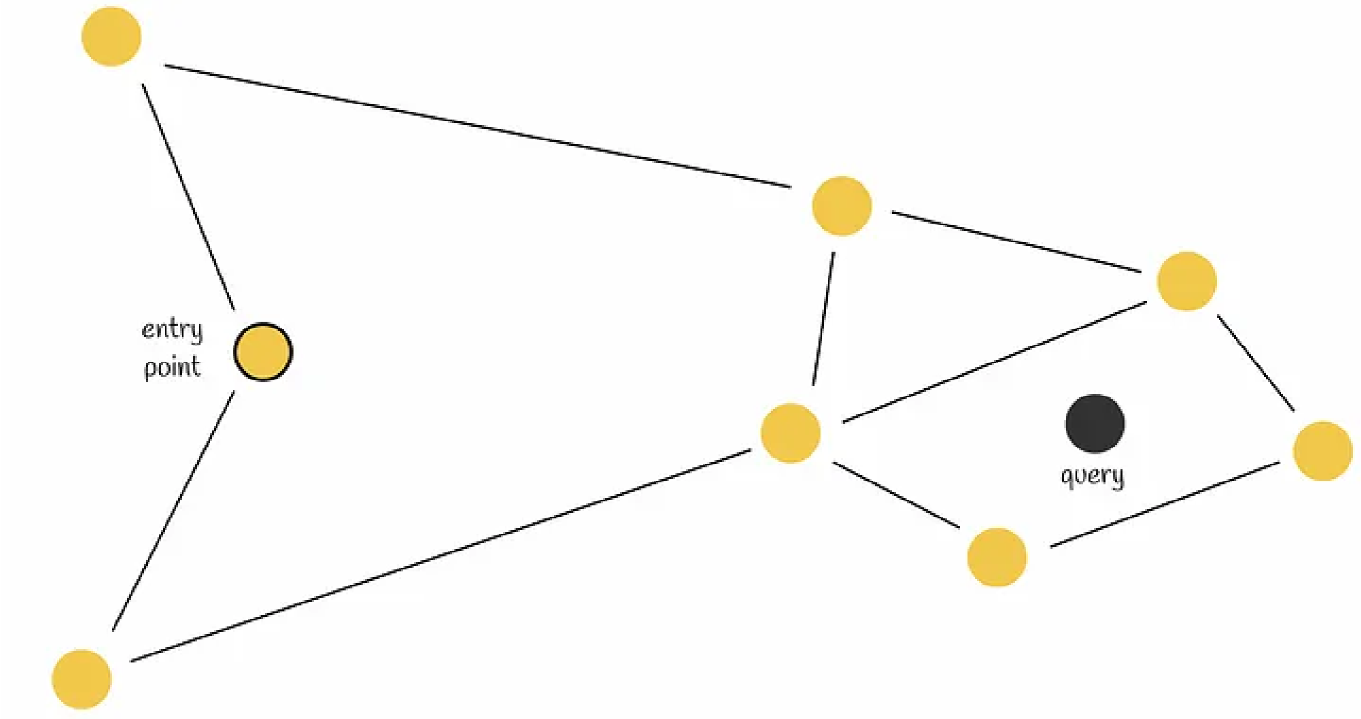
Search

In the first place, search is proceeded by choosing an entry point. To determine the next vertex (or vertices) to which the algorithm makes a move, it calculates the distances from the query vector to the current vertex's neighbours and moves to the closest one. At some point, the algorithm terminates the search procedure when it cannot find a neighbour node that is closer to the query than the current node itself. This node is returned as the response to the query.



Greedy search process in a navigable small world. Node A is used as an entry point. It has two neighbours B and D. Node D is closer to the query than B. As a result, we move to D. Node D has three neighbours C, E and F. E is the closest neighbour to the query, so we move to E. Finally, the search process will lead to node L. Since all neighbours of L are located further from the query than L itself, we stop the algorithm and return L as the answer to the query.

This greedy strategy does not guarantee that it will find the exact nearest neighbour as the method uses only local information at the current step to take decisions. **Early stopping** is one of the problems of the algorithm. It occurs especially at the beginning of the search procedure when there are no better neighbour nodes than the current one. For the most part, this might happen when the starting region has too many low-degree vertices.

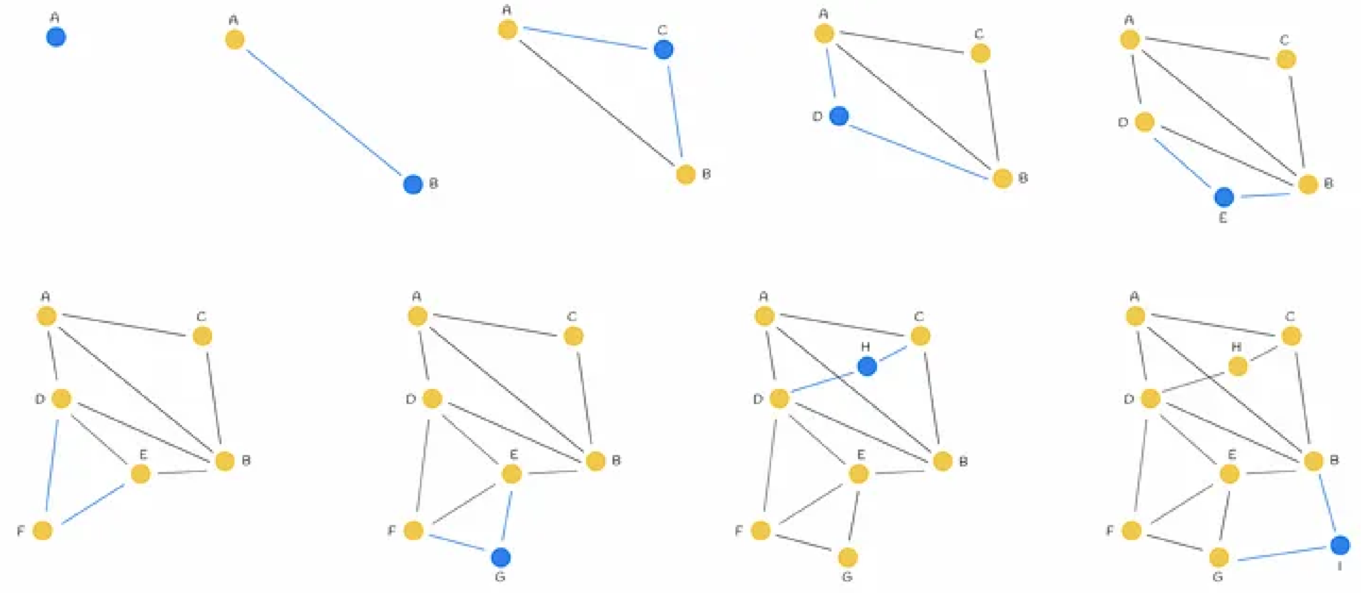


Early stopping. Both neighbours of the current node are further away from the query. Thus, the algorithm returns the current node as the response, though there exist much closer nodes to the query.

The search accuracy can be improved by using several entry points.

Construction

The NSW graph is built by shuffling dataset points and inserting them one by one in the current graph. When a new node is inserted, it is then linked by edges to the M nearest vertices to it.



Sequential insertion of nodes (from left to right) with M = 2. At each iteration, a new vertex is added to the graph and linked to its M = 2 nearest neighbours. Blue lines represent the connected edges to a newly inserted node.

In most scenarios, long-range edges will likely be created at the beginning phase of the graph construction. They play an important role in graph navigation.

> Links to the closest neighbors of the elements inserted in the beginning of the construction later become bridges between the network hubs that keep the overall graph connectivity and allow the logarithmic scaling of the number of hops during greedy routing. — Yu. A. Malkov, D. A. Yashunin

From the example in the figure above, we can see the importance of the long-range edge *AB* that was added in the beginning. Imagine a query requiring the traverse of a path from the relatively far-located nodes *A* and I.

Having the edge *AB* allows doing it rapidly by directly navigating from one side of the graph to the opposite one.

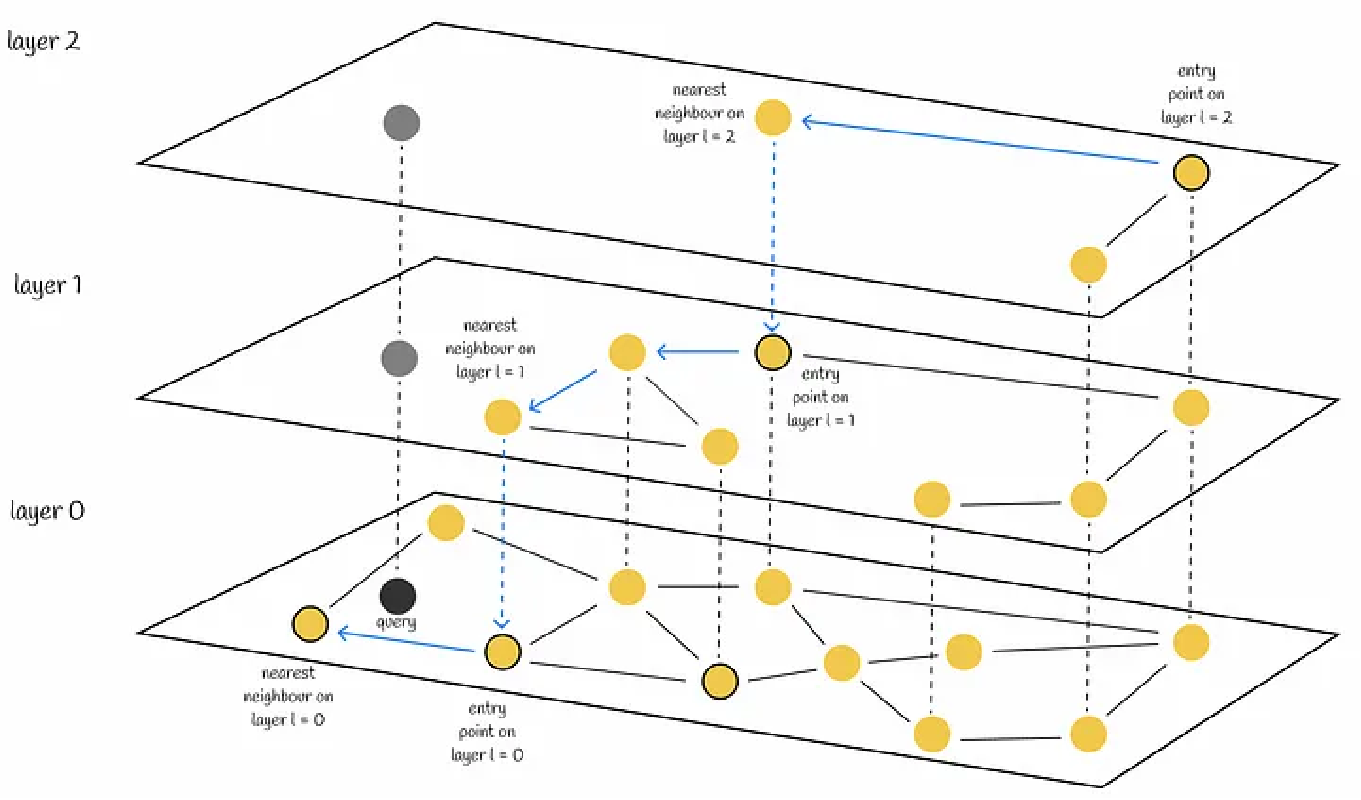
As the number of vertices in the graph increases, it increases the probability that the lengths of newly connected edges to a new node will be smaller.

HNSW

HNSW is based on the same principles as skip list and navigable small world. Its structure represents a multi-layered graph with fewer connections on the top layers and more dense regions on the bottom layers.

Search

The search starts from the highest layer and proceeds to one level below every time the local nearest neighbour is greedily found among the layer nodes. Ultimately, the found nearest neighbour on the lowest layer is the answer to the query.


layer 2
layer 1
layer 0
nearest neighbour on layer l = 2
entry point on layer l = 2
nearest neighbour on layer l = 1
entry point on layer l = 1
query
nearest neighbour on layer l = 0
entry point on layer l = 0

Search in HNSW

Similarly to NSW, the search quality of HNSW can be improved by using several entry points. Instead of finding only one nearest neighbour on each layer, the *efSearch* (a hyperparameter) closest nearest neighbours to the query vector are found and each of these neighbours is used as the entry point on the next layer.

Complexity

The authors of the original paper claim that the number of operations required to find the nearest neighbour on any layer is bounded by a constant. Taking into consideration that the number of all layers in a graph is logarithmic, we get the total search complexity which is *O(logn)*.

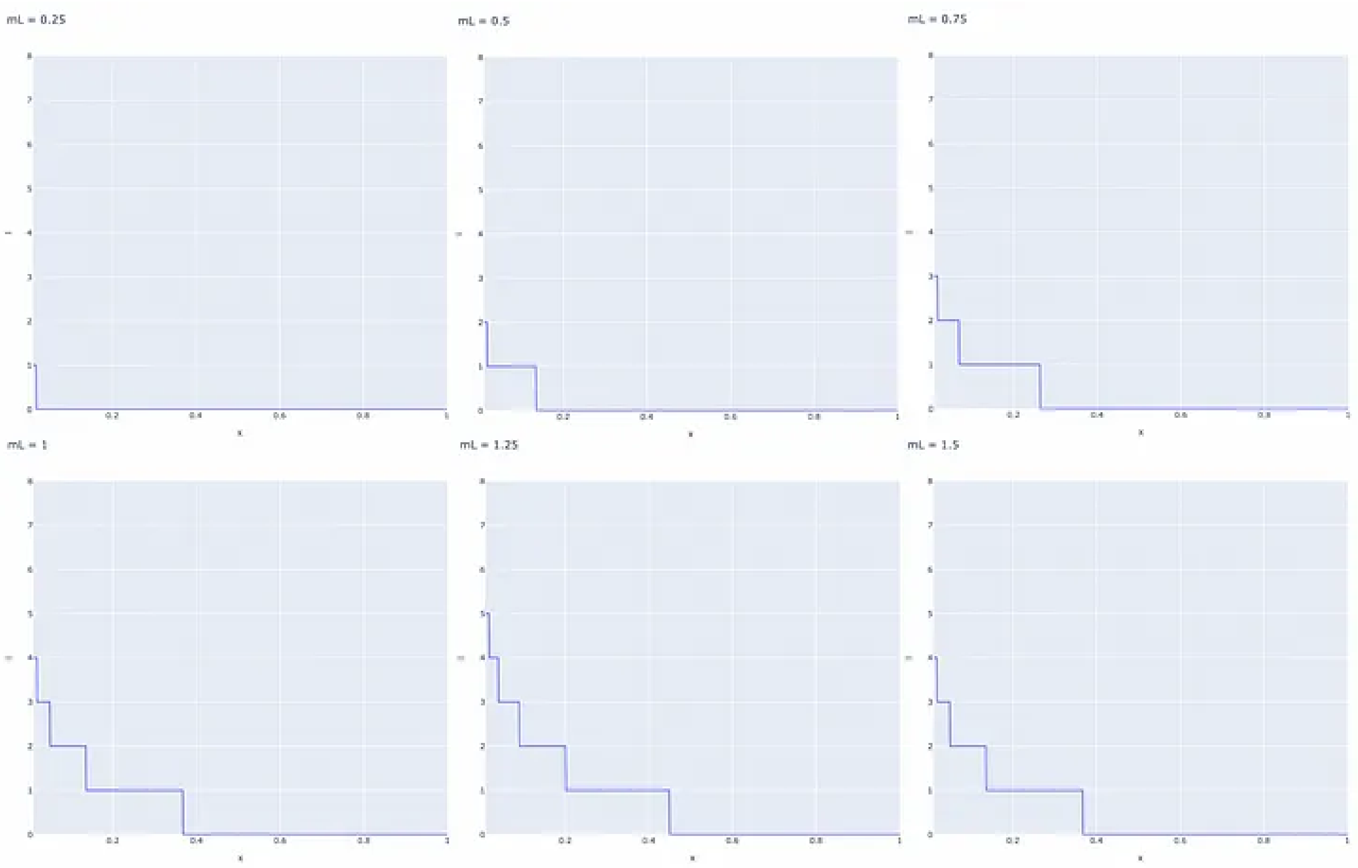
Construction

Choosing the maximum layer

Nodes in HNSW are inserted sequentially one by one. Every node is randomly assigned an integer *l* indicating the maximum layer at which this node can present in the graph. For example, if *l = 1*, then the node can only be found on layers 0 and 1. The authors select *l* randomly for each node with an *exponentially decaying probability distribution* normalized by the non-zero multiplier *mL (mL = 0* results in a single layer in HNSW and non-optimized search complexity*)*. Normally, the majority of *l* values should be equal to 0, so most of the nodes are present only on the lowest level. The larger values of *mL* increase the probability of a node appearing on higher layers.

$$l = \lfloor -\ln(\text{uniform}(0, 1)) \cdot m_L \rfloor$$

The number of layers l for every node is chosen randomly with exponentially decaying probability distribution.



Distribution of the number of layers based on normalization factor mL. The horizontal axis represents values of the uniform(0, 1) distribution.

> To achieve the optimum performance advantage of the controllable hierarchy, the overlap between neighbors on different layers (i.e. percent of element neighbors that are also belong to other layers) has to be small. — Yu. A. Malkov, D. A. Yashunin.

One of the ways to decrease the overlap is to decrease *mL*. But it is important to keep in mind that reducing *mL* also leads on average to more traversals during a greedy search on each layer. That is why it is essential to choose such a value of *mL* that will balance both the overlap and the number of traversals.

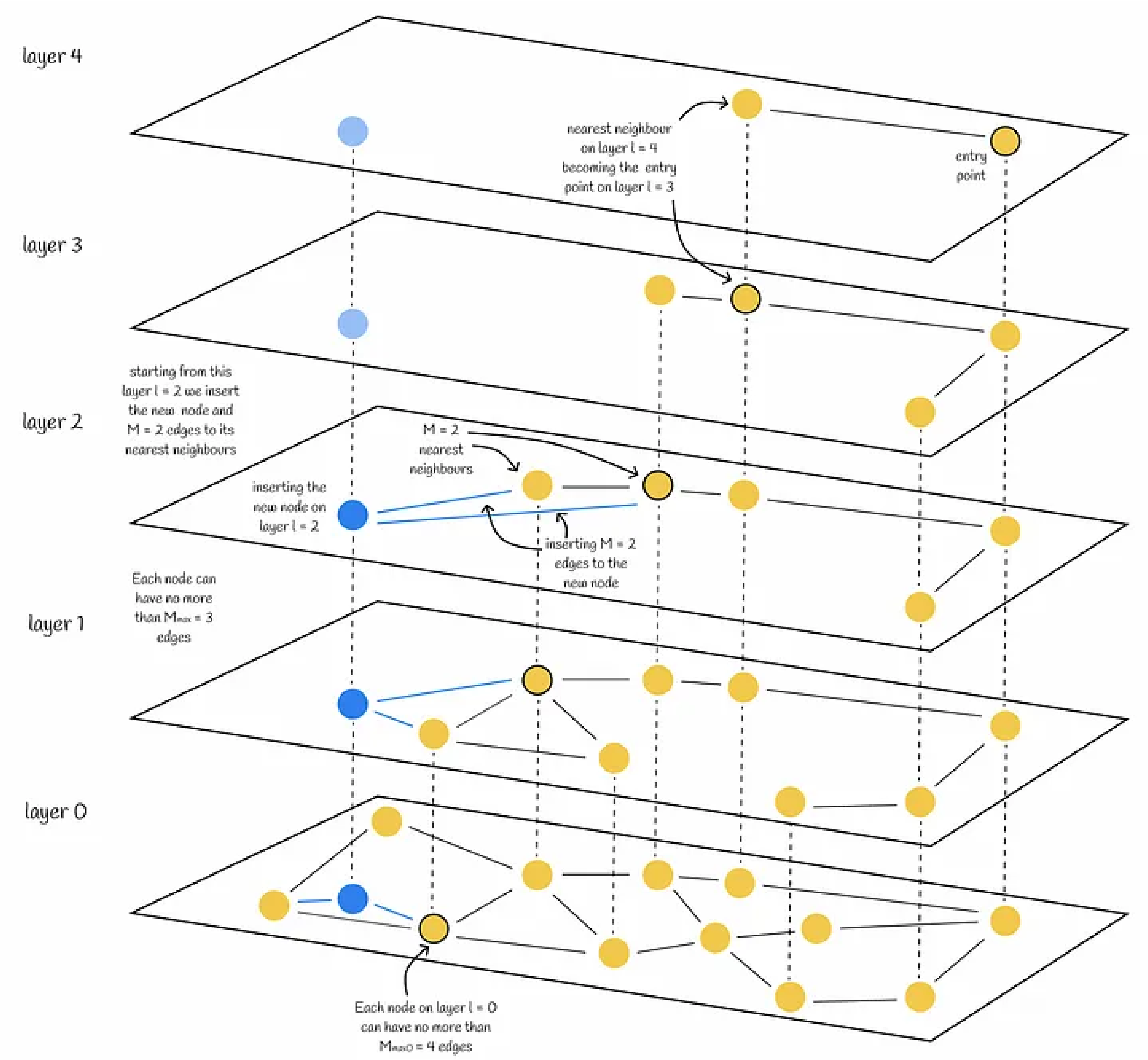
The authors of the paper propose choosing the optimal value of *mL* which is equal to *1 / ln(M)*. This value corresponds to the parameter *p = 1 / M* of the skip list being an average single element overlap between the layers.

Insertion

After a node is assigned the value *l*, there are two phases of its insertion:

1. The algorithm starts from the upper layer and greedily finds the nearest node. The found node is then used as an entry point to the next layer and the search process continues. Once the layer *l* is reached*,* the insertion proceeds to the second step.
2. Starting from layer *l* the algorithm inserts the new node at the current layer. Then it acts the same as before at step 1 but instead of finding only one nearest neighbour, it greedily searches for *efConstruction*

(hyperparameter) nearest neighbours. Then *M* out of *efConstruction* neighbours are chosen and edges from the inserted node to them are built. After that, the algorithm descends to the next layer and each of found *efConstruction* nodes acts as an entry point. The algorithm terminates after the new node and its edges are inserted on the lowest layer 0.


layer 4
nearest neighbour on layer l = 4 becoming the entry point on layer l = 3
entry point
layer 3
starting from this layer l = 2 we insert the new node and M = 2 edges to its nearest neighbours
layer 2
M = 2 nearest neighbours
inserting the new node on layer l = 2
inserting M = 2 edges to the new node
Each node can have no more than M_{max} = 3 edges
layer 1
layer 0
Each node on layer l = 0 can have no more than M_{max0} = 4 edges

Insertion of a node (in blue) in HNSW. The maximum layer for a new node was randomly chosen as l = 2. Therefore, the node will be inserted on layers 2, 1 and 0. On each of these layers, the node will be connected to its M = 2 nearest neighbours.

Choosing values for construction parameters

The original paper provides several useful insights on how to choose hyperparameters:

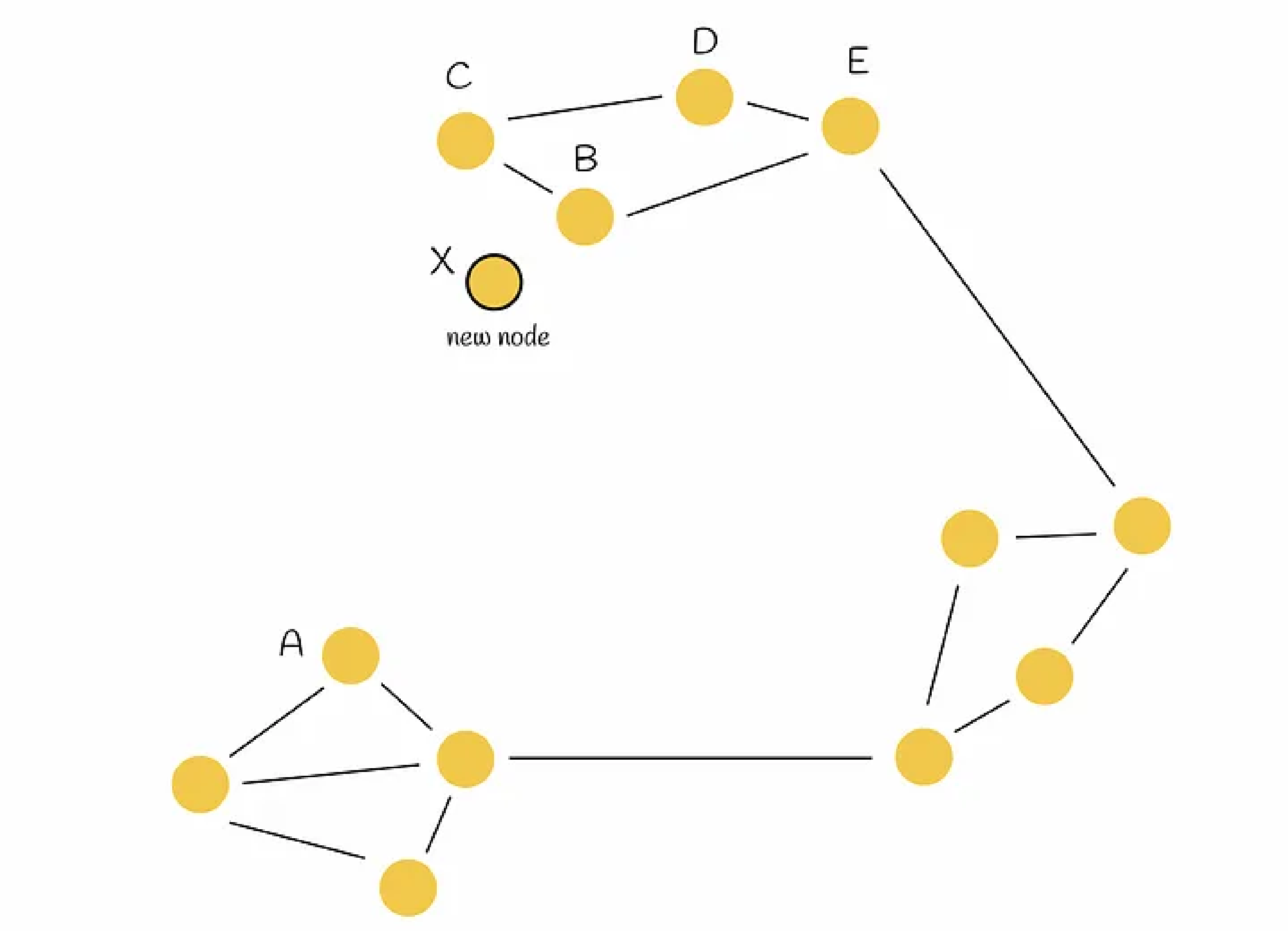
- According to simulations, good values for *M* lie between 5 and 48. Smaller values of *M* tend to be better for lower recalls or low-dimensional data while higher values of M are suited better for high recalls or high-dimensional data.
- Higher values of *efConstruction* imply a more profound search as more candidates are explored. However, it requires more computations. Authors recommend choosing such an *efConstruction* value that results at recall being close to *0.95–1* during training.
- Additionally, there is another important parameter M_{max} — the maximum number of edges a vertex can have. Apart from it, there exists the same parameter M_{max0} but separately for the lowest layer. It is recommended to choose a value for M_{max} close to *2 * M*. Values greater than *2 * M* can lead to performance degradation and excessive memory usage. At the same time, $M_{max} = M$ results in poor performance at high recall.

Candidate selection heuristic

It was noted above that during node insertion, *M* out of *efConstruction* candidates are chosen to build edges to them. Let us discuss possible ways of choosing these *M* nodes.

The naïve approach takes *M* closest candidates. Nevertheless, it is not always the optimal choice. Below is an example demonstrating it.

Imagine a graph with the structure in the figure below. As you can see, there are three regions with two of them not being connected to each other (on the left and on the top). As a result, getting, for example, from point *A* to *B* requires a long path through another region. It would be logical to somehow connect these two regions for better navigation.



Node X is inserted into the graph. The objective is to optimally connect it to other M = 2 points.

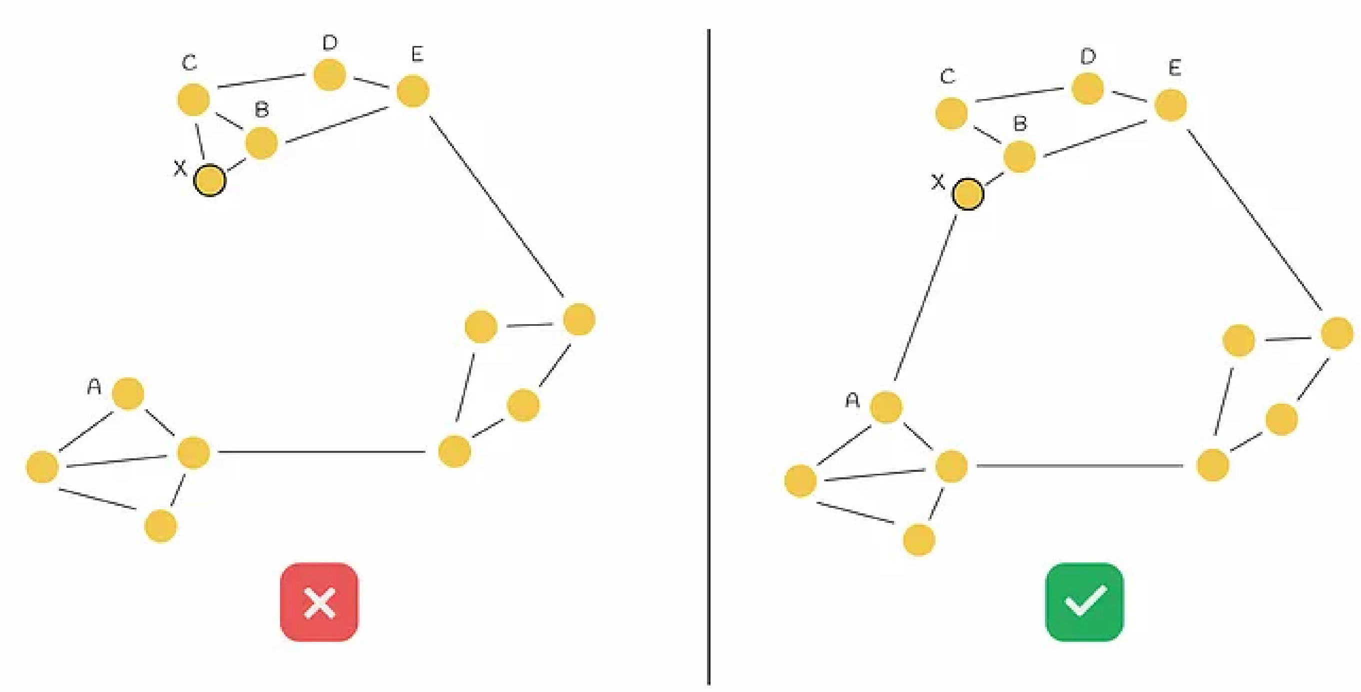
Then a node *X* is inserted into the graph and needs to be linked to *M = 2* other vertices.

In this case, the naïve approach directly takes the *M = 2* nearest neighbours (*B* and *C*) and connects *X* to them. Though *X* is connected to its real nearest neighbours, it does not solve the problem. Let us look at the heuristical approach invented by the authors.

> The heuristic considers not only the closest distances between nodes but also the connectivity of different regions on the graph.

The heuristic chooses the first nearest neighbour (*B* in our case) and connects the inserted node (*X*) to it. Then the algorithm sequentially takes another most closest nearest neighbour in the sorted order (*C*) and builds an edge to it only if the distance from this neighbour to the new node (*X*) is smaller than any distance from this neighbour to all already connected vertices (*B*) to the new node (*X*). After that, the algorithm proceeds to the next closest neighbour until *M* edges are built.

Getting back to the example, the heuristical procedure is illustrated in the figure below. The heuristic chooses *B* as the closest nearest neighbour for X and builds the edge *BX*. Then the algorithm chooses *C* as the next closest nearest neighbour. However, this time $BC < CX$. This indicates that adding the edge *CX* to the graph is not optimal because there already exists the edge *BX* and the nodes *B* and *C* are very close to each other. The same analogy proceeds with the nodes *D* and *E*. After that, the algorithm examines the node *A*. This time, it satisfies the condition since $BA > AX$. As a result, the new edge *AX* and both initial regions become connected to each other.



The example on the left uses the naïve approach. The example on the right uses the selection heuristic which results in two initial disjoint regions being connected to each other.

Complexity

The insertion process works very similarly, compared to the search procedure, without any significant differences which could require a non-constant number of operations. Thus, the insertion of a single vertex imposes *O(logn)* of time. To estimate the total complexity, the number of all inserted nodes *n* in a given dataset should be considered. Ultimately, HNSW construction requires *O(n * logn)* time.

Combining HNSW with other methods

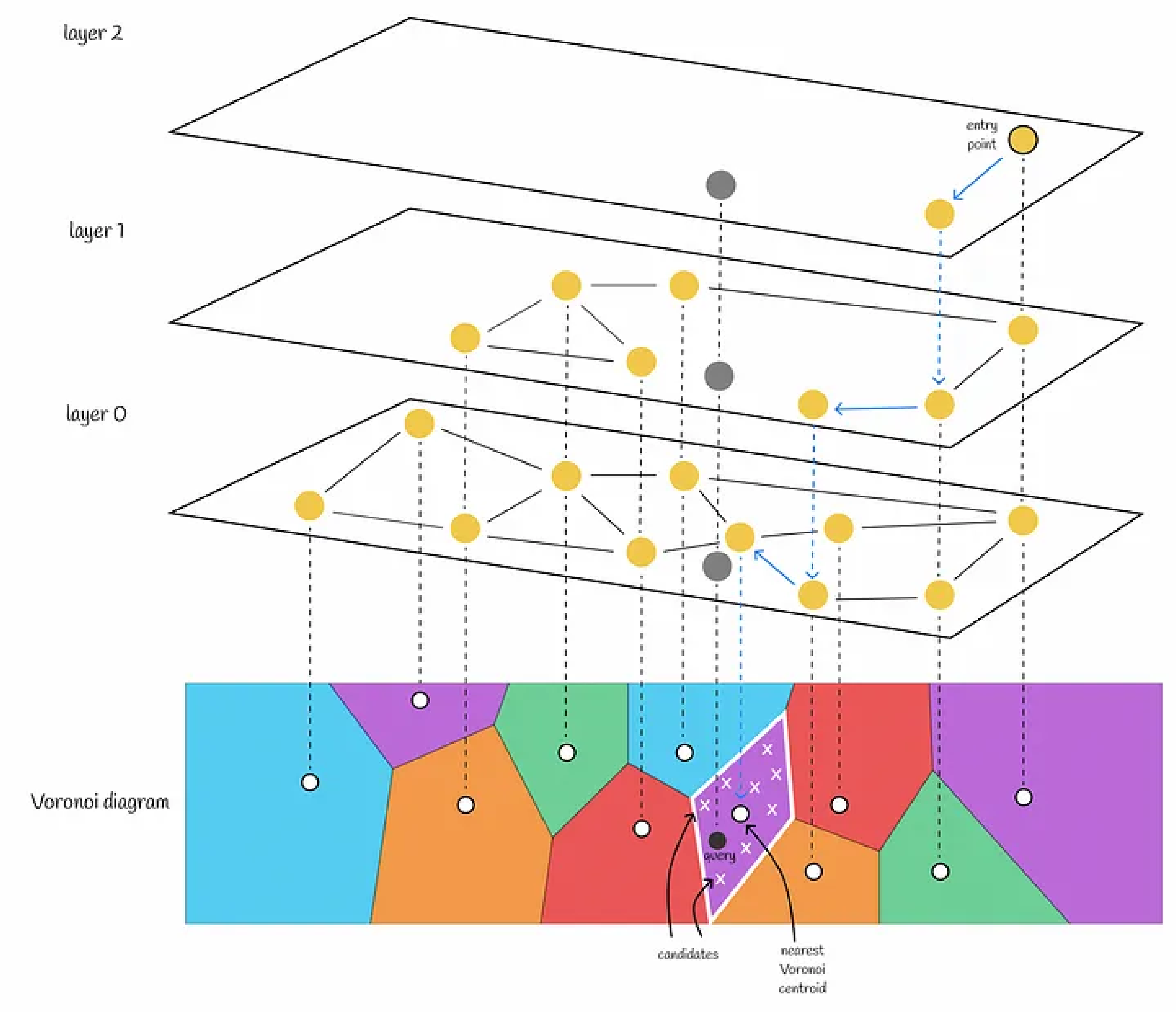
HNSW can be used together with other similarity search methods to provide better performance. One of the most popular ways to do it is to combine it with an inverted file index and product quantization (*IndexIVFPQ*) which were described in other parts of this article series.

Similarity Search, Part 3: Blending Inverted File Index and Product Quantization

In the first two parts of this series we have discussed two fundamental algorithms in information retrieval: inverted…

medium.com

Within this paradigm, HNSW plays the role of a **coarse quantizer** for *IndexIVFPQ* meaning that it will be responsible for finding the nearest Voronoi partition, so the search scope can be reduced. To do it, an HNSW index has to be built on all Voronoi centroids. When given a query, HNSW is used to find the nearest Voronoi centroid (instead of brute-force search as it was previously by comparing distances to every centroid). After that, the query vector is quantized within a respective Voronoi partition and distances are calculated by using PQ codes.



Choosing the nearest Voronoi centroid by finding the nearest neighbour in HNSW built on top of Voronoi centroids.

When using only an inverted file index, it is better to set the number of Voronoi partitions not too large (256 or 1024, for instance) because brute-force search is performed to find the nearest centroids. By choosing a small number of Voronoi partitions, the number of candidates inside each partition becomes relatively large. Therefore, the algorithm rapidly identifies the nearest centroid for a query and most of its runtime is concentrated on finding the nearest neighbour inside a Voronoi partition.

However, introducing HNSW into the workflow requires an adjustment. Consider running HNSW only on a small number of centroids (256 or 1024): HNSW would not bring any significant benefits because, with a small number of vectors, HNSW performs relatively the same in terms of execution time as naïve brute-force search. Moreover, HNSW would require more memory to store the graph structure.

> *That is why when merging HNSW and inverted file index, it is recommended to set the number of Voronoi centroids much bigger than usual. By doing so, the number of candidates inside each Voronoi partition becomes much smaller.*

This shift in paradigm results in the following settings:

- HNSW rapidly identifies the nearest Voronoi centroids in logarithmic time.
- After that, an exhaustive search inside respective Voronoi partitions is performed. It should not be a trouble because the number of potential candidates is small.

Faiss implementation

> ***Faiss*** *(Facebook AI Search Similarity) is a Python library written in C++ used for optimised similarity search. This library presents different types of indexes which are data structures used to efficiently store the data and perform queries.*

Based on the information from the Faiss documentation, we will see how HNSW can be utilized and merged together with inverted file index and product quantization.

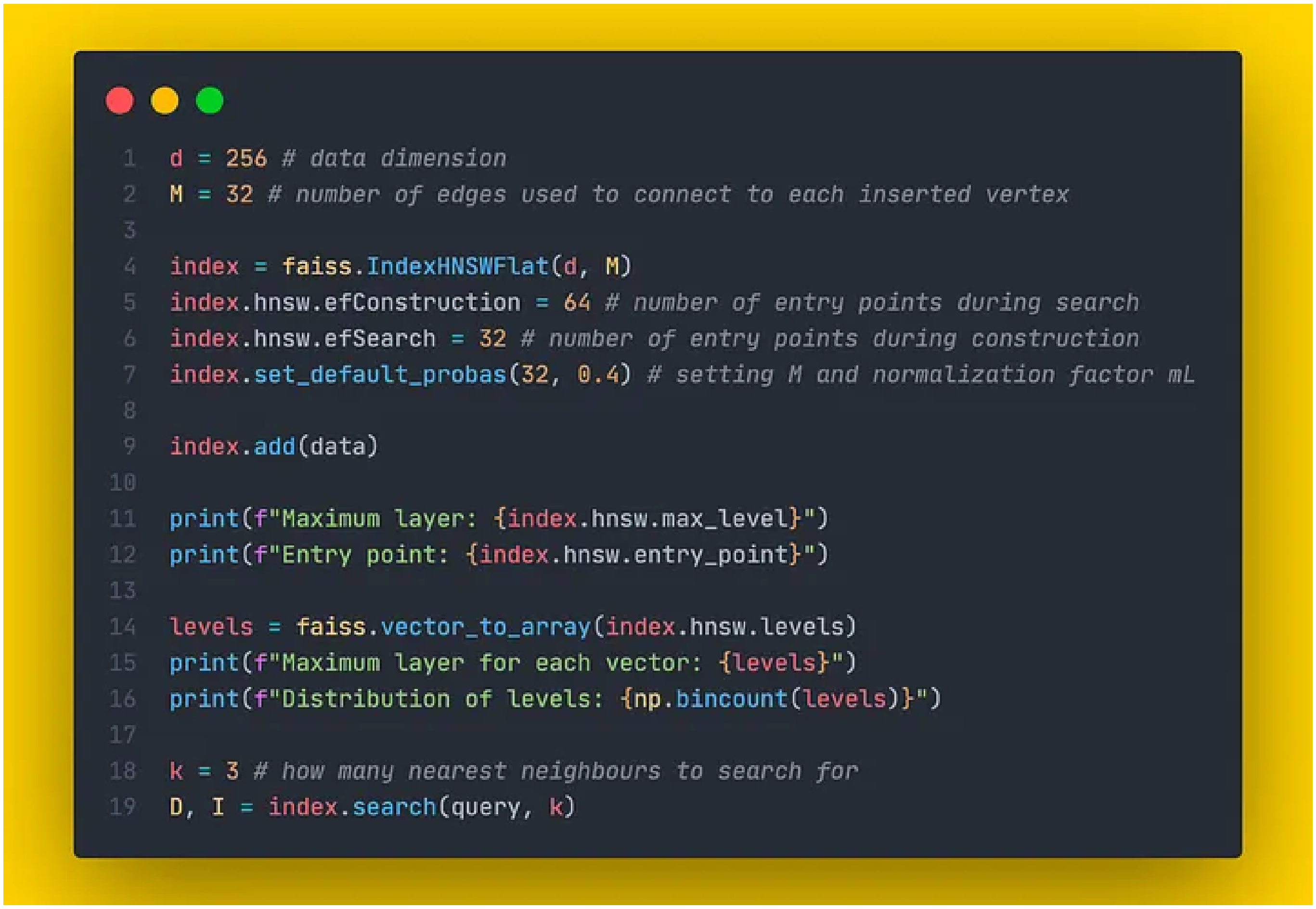
IndexHNSWFlat

FAISS has a class *IndexHNSWFlat* implementing the HNSW structure. As usual, the suffix "*Flat*" indicates that dataset vectors are fully stored in index. The constructor accepts 2 parameters:

- **d**: data dimensionality.
- **M**: the number of edges that need to be added to every new node during insertion.

Additionally, via thr **hnsw** field*, IndexHNSWFlat* provides several useful attributes (which can be modified) and methods:

- **hnsw.efConstruction:** number of nearest neighbours to explore during construction.
- **hnsw.efSearch**: number of nearest neighbours to explore during search.
- **hnsw.max_level**: returns the maximum layer.
- **hnsw.entry_point**: returns the entry point.
- **faiss.vector_to_array(index.hnsw.levels):** returns a list of maximum layers for each vector
- **hnsw.set_default_probas(M: int, level_mult: float):** allows setting *M* and *mL* values respectively. By default*, level_mult* is set to *1 / ln(M)*.



```
d = 256 # data dimension
M = 32 # number of edges used to connect to each inserted vertex

index = faiss.IndexHNSWFlat(d, M)
index.hnsw.efConstruction = 64 # number of entry points during search
index.hnsw.efSearch = 32 # number of entry points during construction
index.set_default_probas(32, 0.4) # setting M and normalization factor mL

index.add(data)

print(f"Maximum layer: {index.hnsw.max_level}")
print(f"Entry point: {index.hnsw.entry_point}")

levels = faiss.vector_to_array(index.hnsw.levels)
print(f"Maximum layer for each vector: {levels}")
print(f"Distribution of levels: {np.bincount(levels)}")

k = 3 # how many nearest neighbours to search for
D, I = index.search(query, k)
```

Faiss implementation of IndexHNSWFlat

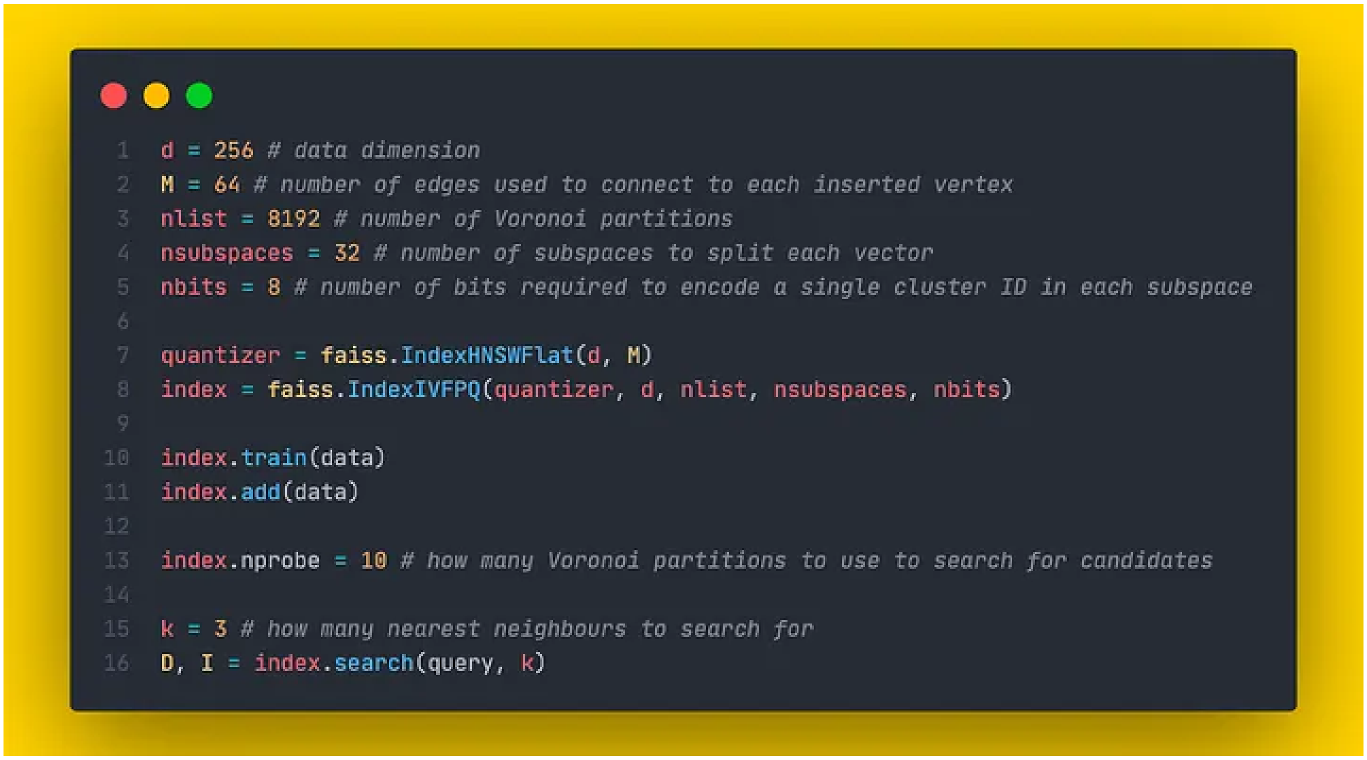
IndexHNSWFlat sets values for $M_{max} = M$ and $M_{max0} = 2 * M$.

IndexHNSWFlat + IndexIVFPQ

IndexHNSWFlat can be combined with other indexes as well. One of the examples is *IndexIVFPQ* described in the previous part. Creation of this composite index proceeds in two steps:

1. *IndexHNSWFlat* is initialized as a coarse quantizer.
2. The quantizer is passed as a parameter to the constructor of *IndexIVFPQ*.

Training and adding can be done by using different or the same data.



```python
d = 256 # data dimension
M = 64 # number of edges used to connect to each inserted vertex
nlist = 8192 # number of Voronoi partitions
nsubspaces = 32 # number of subspaces to split each vector
nbits = 8 # number of bits required to encode a single cluster ID in each subspace

quantizer = faiss.IndexHNSWFlat(d, M)
index = faiss.IndexIVFPQ(quantizer, d, nlist, nsubspaces, nbits)

index.train(data)
index.add(data)

index.nprobe = 10 # how many Voronoi partitions to use to search for candidates

k = 3 # how many nearest neighbours to search for
D, I = index.search(query, k)
```

FAISS implementation of IndexHNSWFlat + IndexIVFPQ

Conclusion

In this article, we have studied a robust algorithm which works especially well for large dataset vectors. By using multi-layer graph representations and the candidate selection heuristic its search speed scales efficiently while maintaining a decent prediction accuracy. It is also worth noting that HNSW can be used in combination with other similarity search algorithms making it very flexible.

Resources

- Six degrees of separation | Wikipedia
- Skip List | Wikipedia
- Efficient and robust approximate nearest neighbor search using Hierarchical Navigable Small World graphs. Yu. A. Malkov, D. A. Yashunin

- Faiss documentation
- Faiss repository
- Summary of Faiss indexes

All images unless otherwise noted are by the author.

Machine Learning · Nearest Neighbors · Faiss · Graph · Similarity Search

More from the list: "NLP"

Curated by Himanshu Birla

Jon Gi... in Towards Data ...

Characteristics of Word Embeddings

✦ · 11 min read · Sep 4, 2021

Jon Gi... in Towards Data ...

The Word2vec Hyperparameters

✦ · 6 min read · Sep 3, 2021

Jon Gi... in

The Word2ve

✦ · 15 min rea

View list

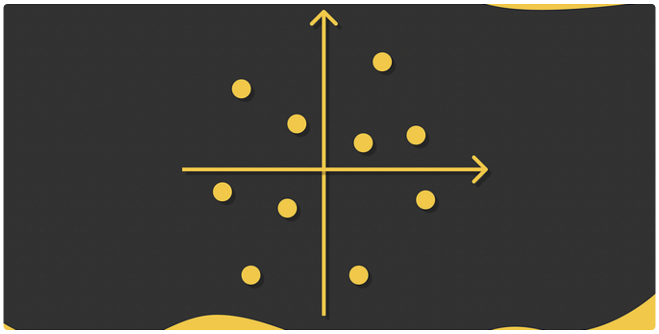
Written by Vyacheslav Efimov

Following

470 Followers · Writer for Towards Data Science

BSc in Software Engineering. Passionate machine learning engineer. Writer at Towards Data Science.

More from Vyacheslav Efimov and Towards Data Science



Vyacheslav Efimov in Towards Data Science

Similarity Search, Part 3: Blending Inverted File Index and Product...

In the first two parts of this series we have discussed two fundamental algorithms in...

8 min read · May 19

128

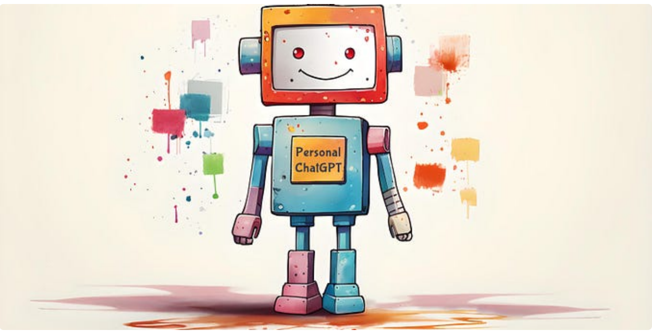
Antonis Makropoulos in Towards Data Science

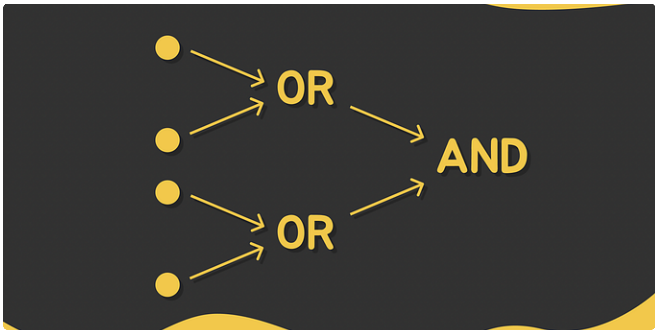
How to Build a Multi-GPU System for Deep Learning in 2023

This story provides a guide on how to build a multi-GPU system for deep learning and...

10 min read · Sep 17

549 11





Robert A. Gonsalves in Towards Data Science

Your Own Personal ChatGPT

How you can fine-tune OpenAI's GPT-3.5 Turbo model to perform new tasks using you...

· 15 min read · Sep 8

595 7

Vyacheslav Efimov in Towards Data Science

Similarity Search, Part 7: LSH Compositions

Dive into combinations of LSH functions to guarantee a more reliable search

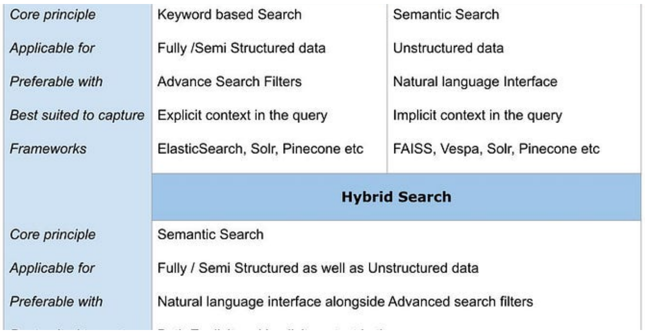
11 min read · Jul 24

43

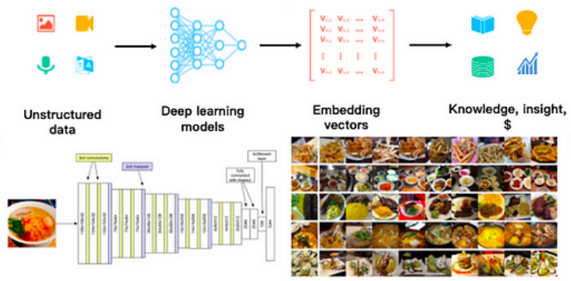
See all from Vyacheslav Efimov

See all from Towards Data Science

Recommended from Medium



Core principle	Keyword based Search	Semantic Search
Applicable for	Fully /Semi Structured data	Unstructured data
Preferable with	Advance Search Filters	Natural language Interface
Best suited to capture	Explicit context in the query	Implicit context in the query
Frameworks	ElasticSearch, Solr, Pinecone etc	FAISS, Vespa, Solr, Pinecone etc
	Hybrid Search	
Core principle	Semantic Search	
Applicable for	Fully / Semi Structured as well as Unstructured data	
Preferable with	Natural language interface alongside Advanced search filters	



Maithri Vm

Hybrid Search — Amalgamation of Sparse and Dense vector…

— Uniting meaning of data with metadata to leverage deeper context

13 min read · May 14

16

Jayita Bhattacharyya in GoPenAI

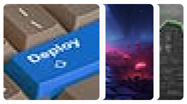
Primer on Vector Databases and Retrieval-Augmented Generation…

Vector Databases Generation (RAG) Langchain Pinecone HuggingFace Large…

9 min read · Aug 16

228 1

Lists

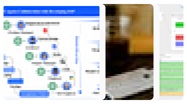


Predictive Modeling w/ Python

20 stories · 452 saves

Practical Guides to Machine Learning

10 stories · 519 saves

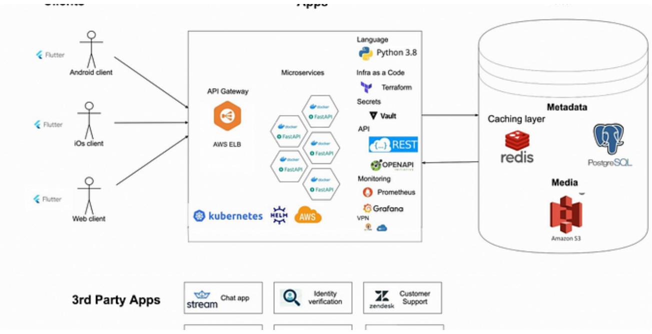


Natural Language Processing

669 stories · 283 saves

The New Chatbots: ChatGPT, Bard, and Beyond

13 stories · 133 saves



Dmitry Kruglov in Better Programming

The Architecture of a Modern Startup

Hype wave, pragmatic evidence vs the need to move fast

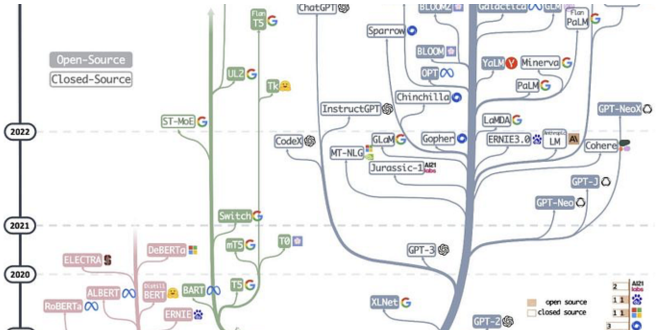
NoCode AI in **AI monks.io**

Understanding Vector Database and Indexing — Visual Guide for…

What is vectors databases? Let's break it down into simple terms and explore it visually.

16 min read · Nov 7, 2022

6.1K 59



Haifeng Li

A Tutorial on LLM

Generative artificial intelligence (GenAI), especially ChatGPT, captures everyone's...

15 min read · Sep 14

372

✦ · 6 min read · May 28

33 1

Alyx

Semantic Search with FAISS

HuggingFace get_neareast_example and Cosine Similarity Search

9 min read · Jul 15

71 1

See more recommendations