Indexing Vectors

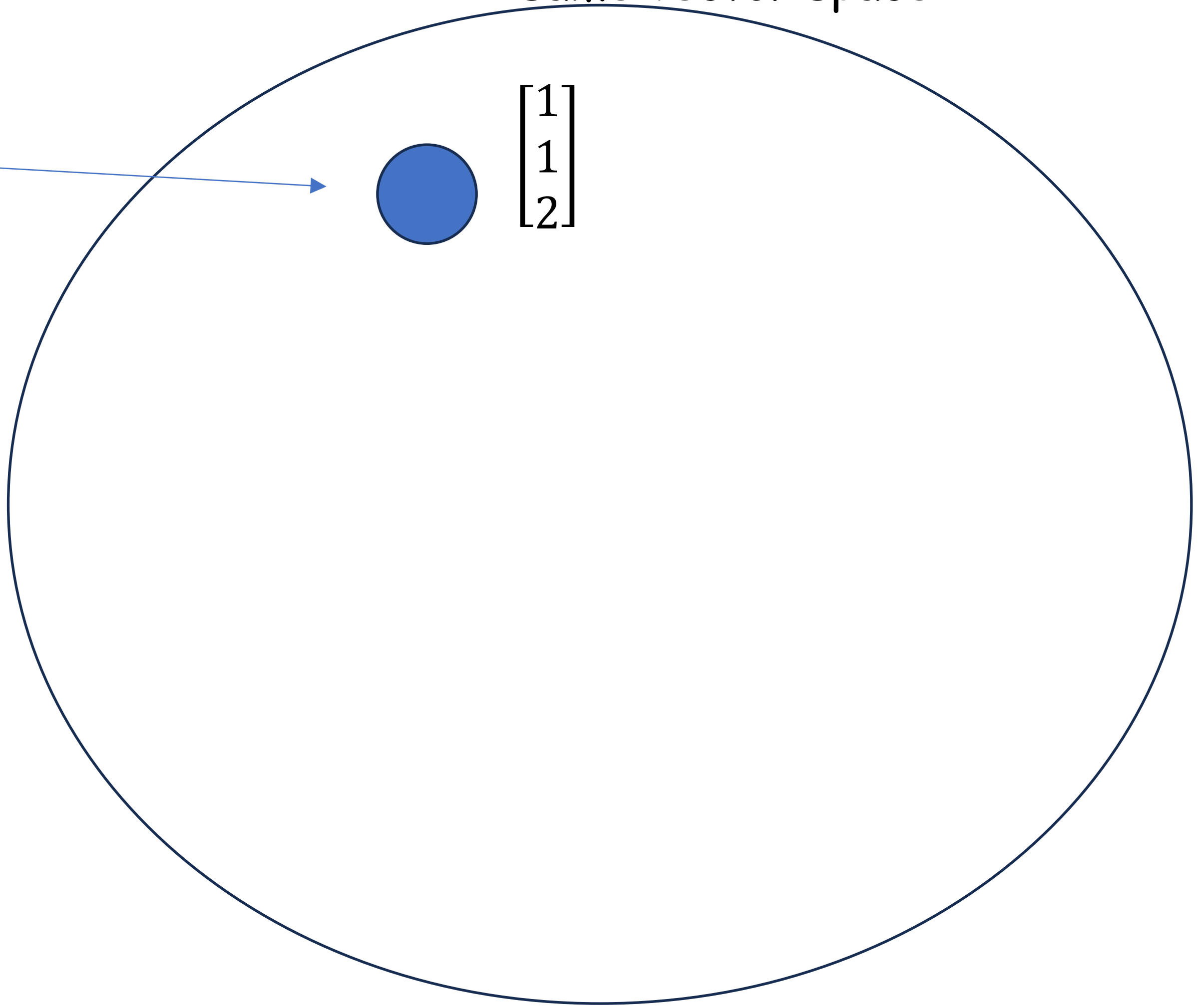
Alfan F. Wicaksono

https://www.pinecone.io/learn/series/faiss/hnsw/

Nowadays, everything can be encoded into vectors (or tensors)

Vector Database
"A collection of vectors from the same vector space"

"Gedung Fasilkom UI"



$$\begin{bmatrix}1\\1\\2\end{bmatrix}$$

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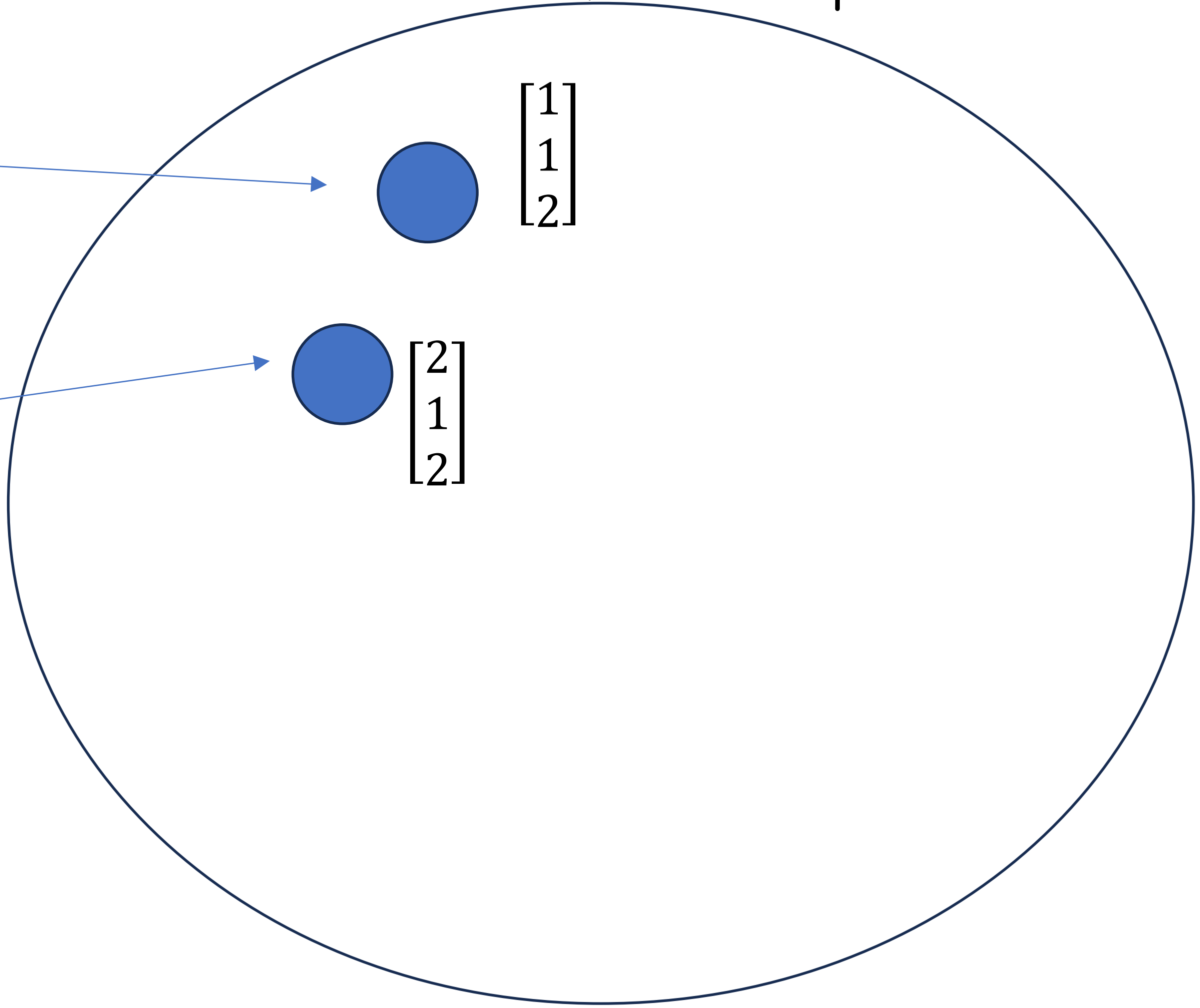

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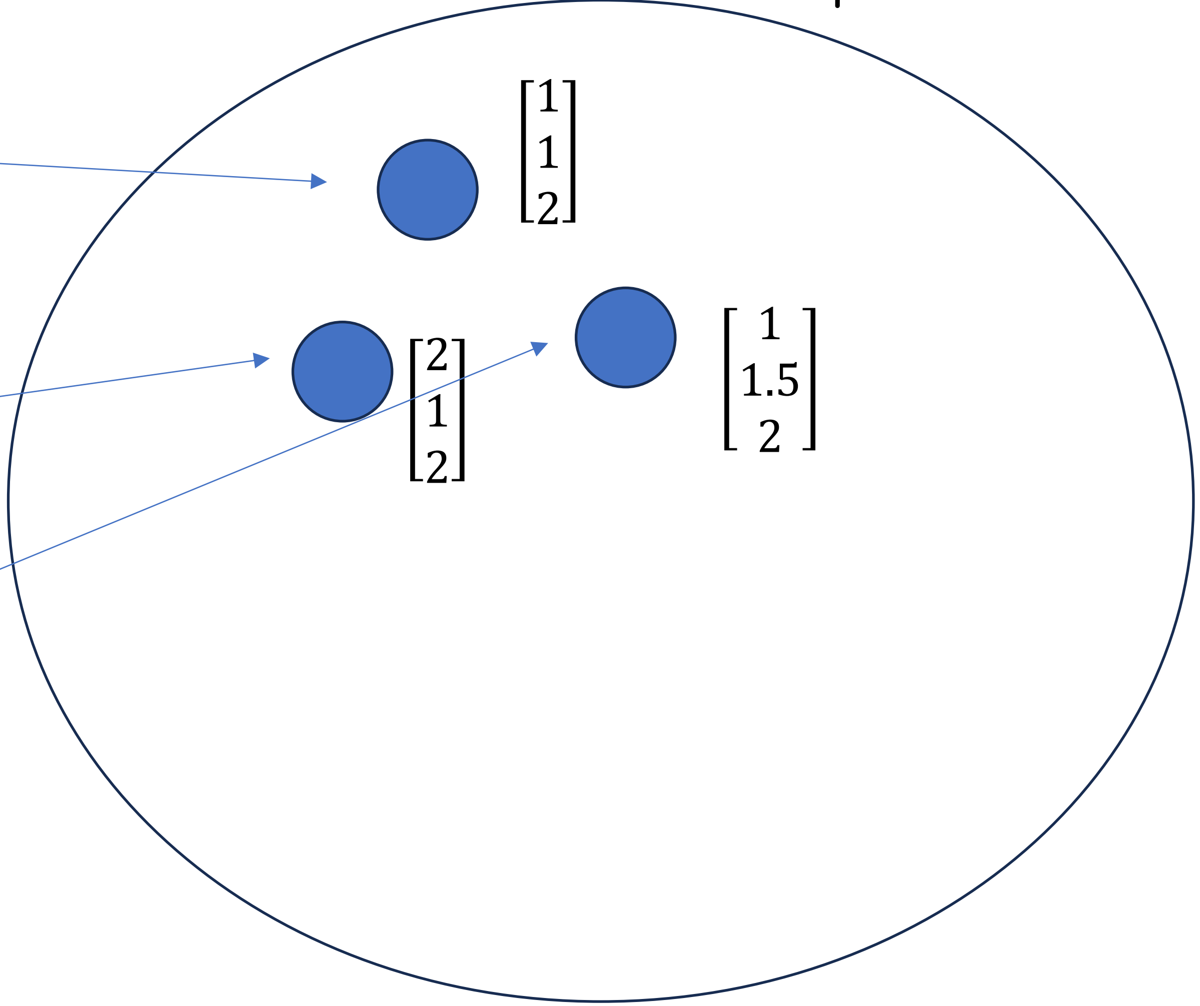
Music: Mars Fasilkom UI



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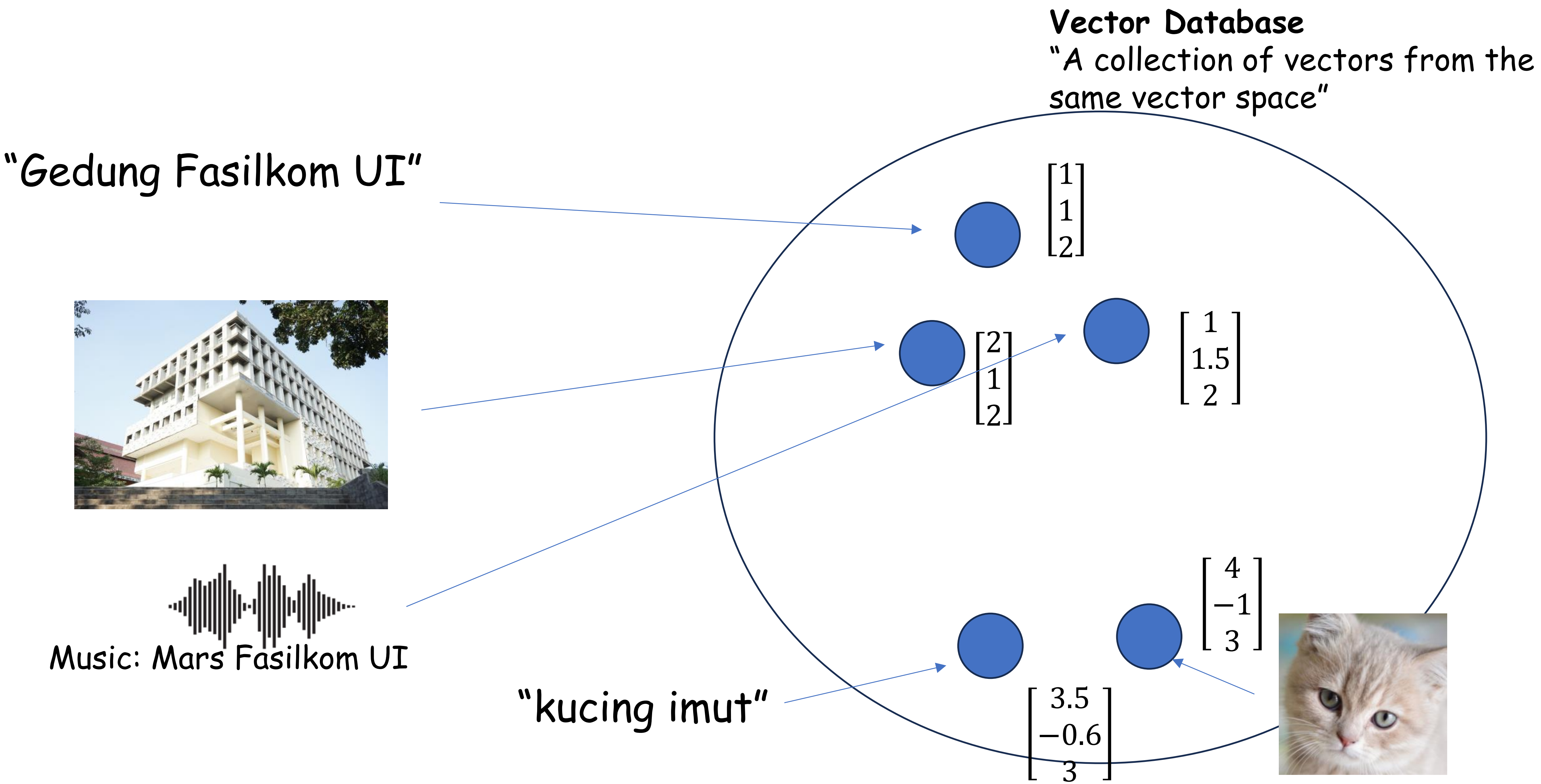
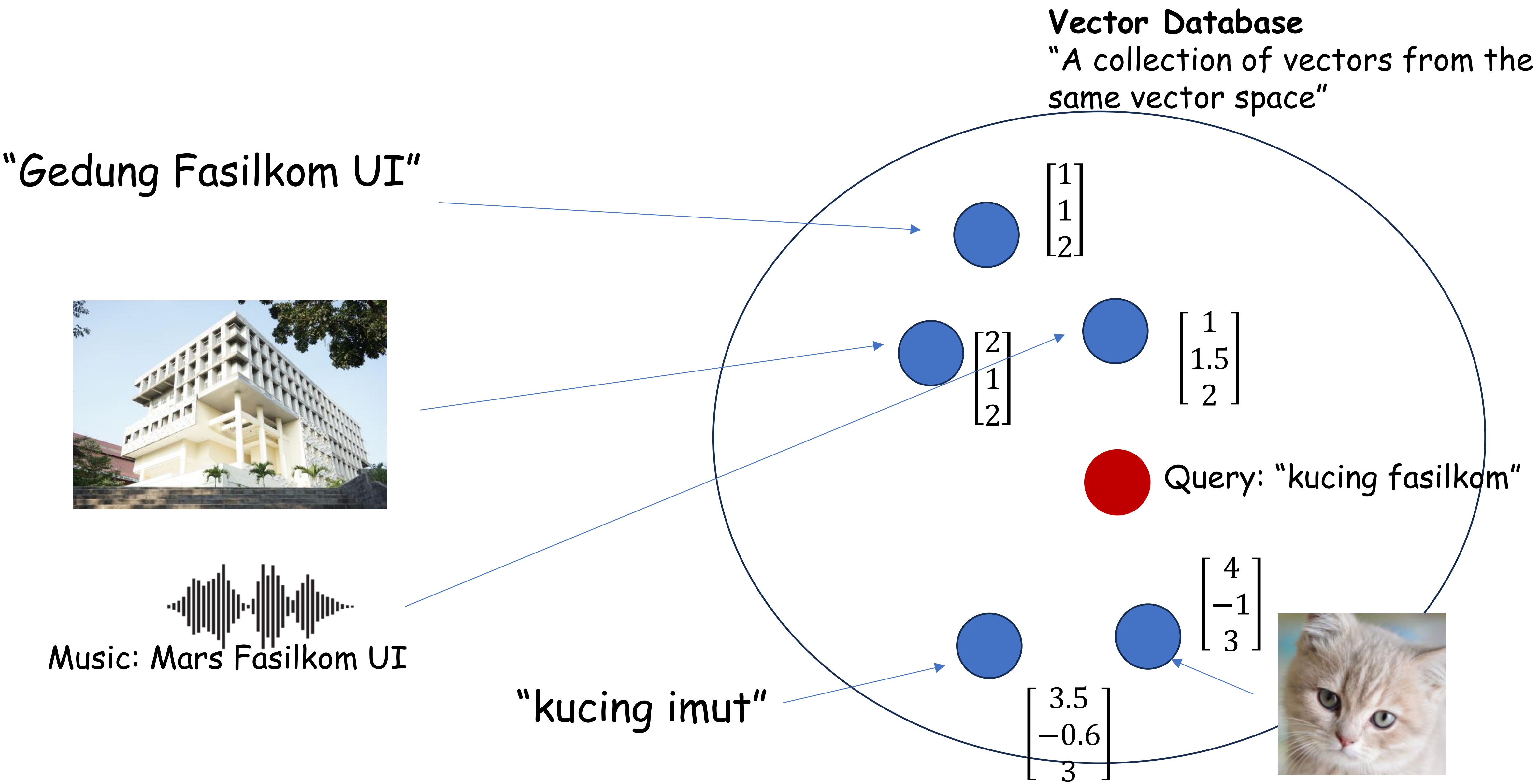


K-Nearest neighbor search

- Given a query (which can be in any format, including text, image, or audio), find other items that are "similar" to the query.
  - Nowadays, everything can be represented as **vectors**!
- Given a set $\boldsymbol{S}$ of points in a space $\boldsymbol{M}$ and a query point $\boldsymbol{q} \in \boldsymbol{M}$, find $\boldsymbol{k}$ closest points in $\boldsymbol{S}$ to $\boldsymbol{q}$.
- $\boldsymbol{M}$ is a **metric space** and similarity is expressed as a distance metric, which is symmetric and satisfies triangle inequality.
  - Euclidean distance (**L2**), Inner Product, Manhattan distance, …

Nowadays, everything can be encoded into vectors (or tensors)



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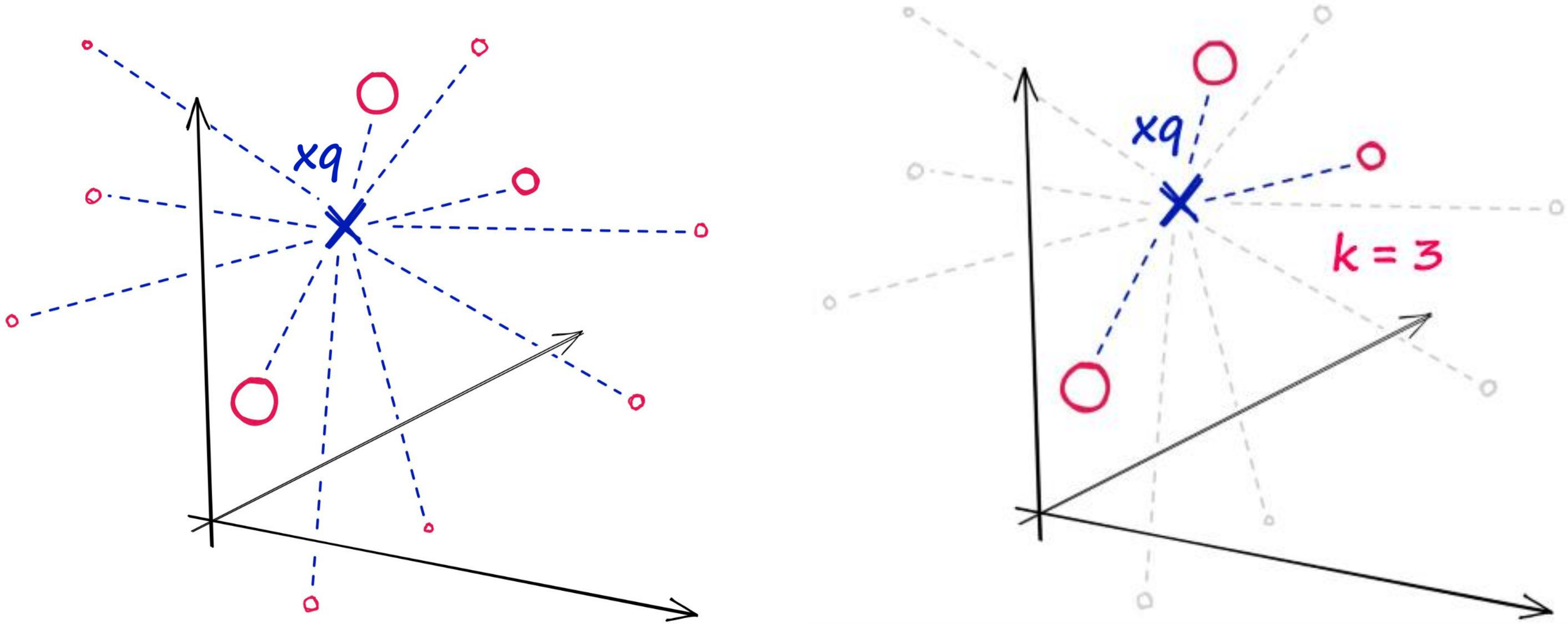
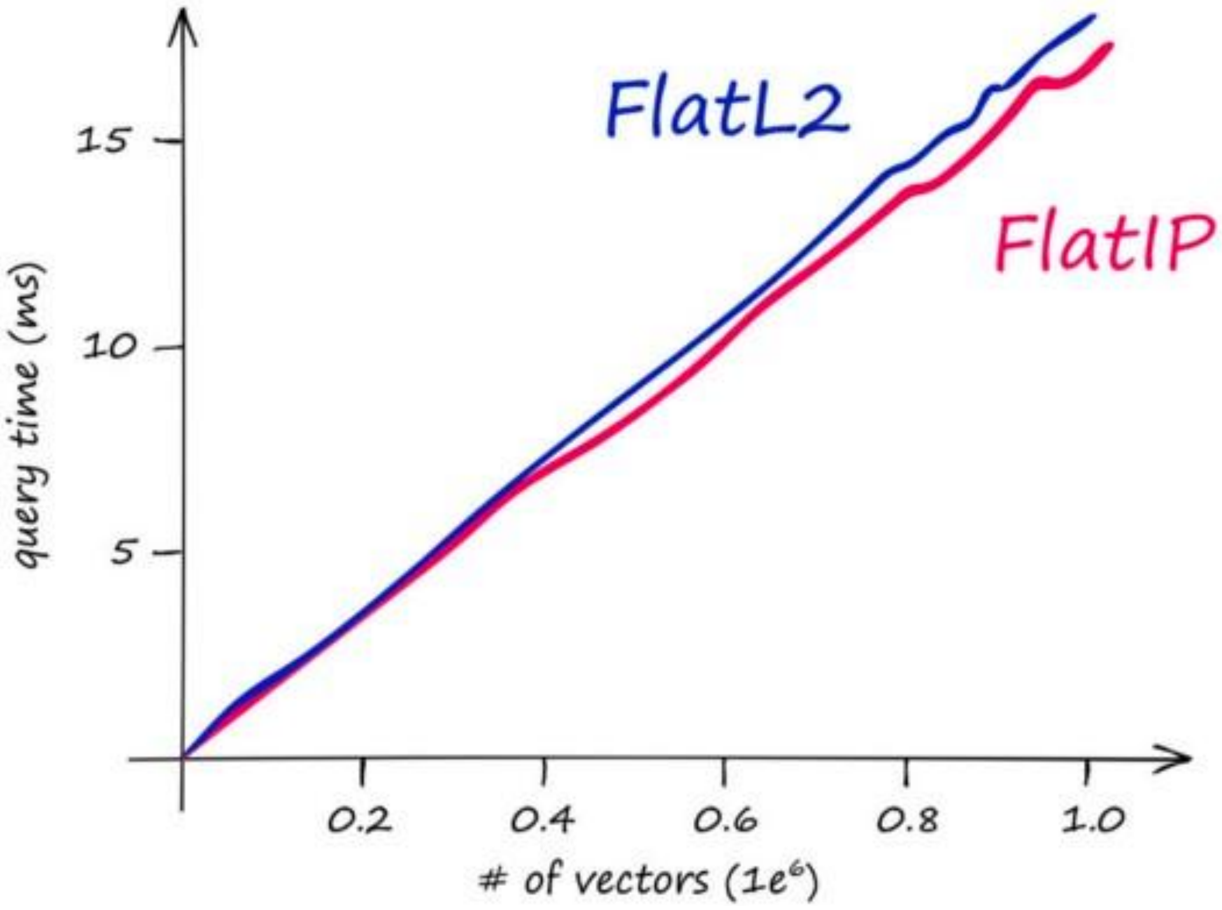
Exact Solution – Flat Index



The query vector **xq** is against every other vectors in the index, calculating the distance to each and returning k nearest points.

https://www.pinecone.io/learn/series/faiss/vector-indexes/

Exact Solution – Flat Index



Tools FAISS: Euclidean (L2) and Inner Product (IP) flat index search times using faiss-cpu on an M1 chip. Both using vector dimensionality of 100. IndexFlatIP is shown to be slightly faster than IndexFlatL2.

https://www.pinecone.io/learn/series/faiss/vector-indexes/

Approximate nearest neighbors

- Flat index is 100% accurate, but slow and not scalable as the number of vectors in the database increases.

- One solution is to **reduce the search scope**.
    - We can somehow cluster and organize vectors into tree structures based on certain attributes or similarities.
    - We are no longer performing an exhaustive nearest-neighbors search but an **approximate nearest-neighbors**.

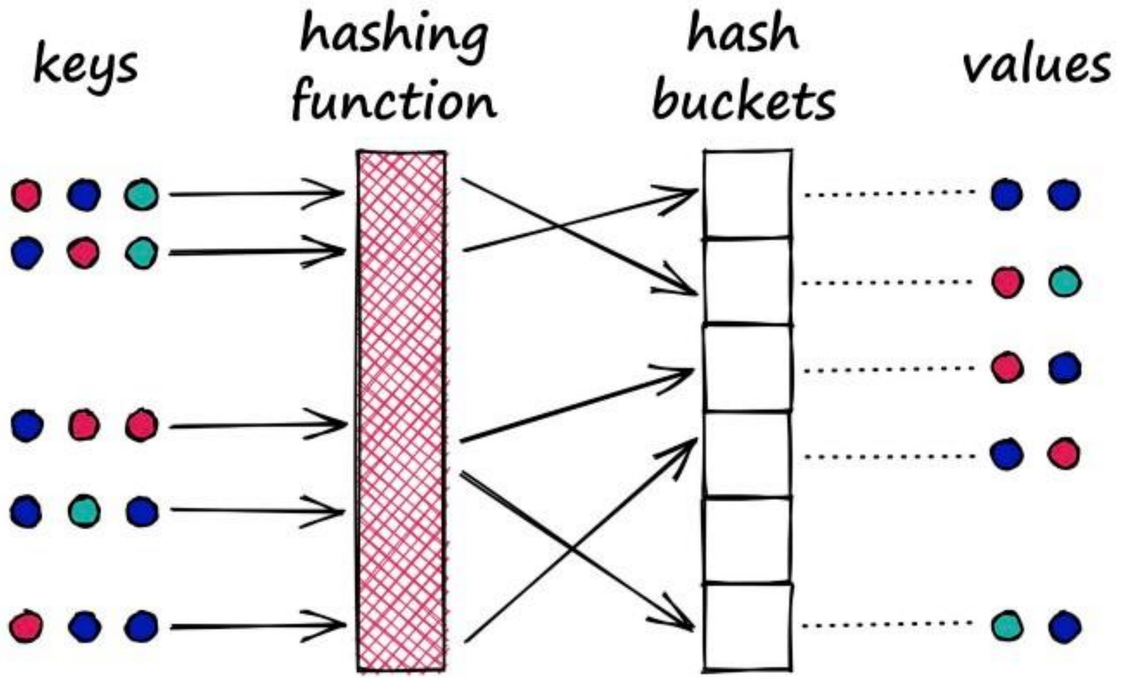
Three Types ANN Algorithms

- Using Trees (e.g. k-d trees)
- **Using Locality Sensitive Hashing (e.g. Random Projection)**
- Using Graphs (Hierarchical Navigable Small Worlds)

https://www.pinecone.io/learn/series/faiss/vector-indexes/

Typical Hashing

- Remember “Hash Table” on your last SDA course!
- We want a hash function that **minimizes collisions**; we really want to have multiple vectors mapped to a single key.



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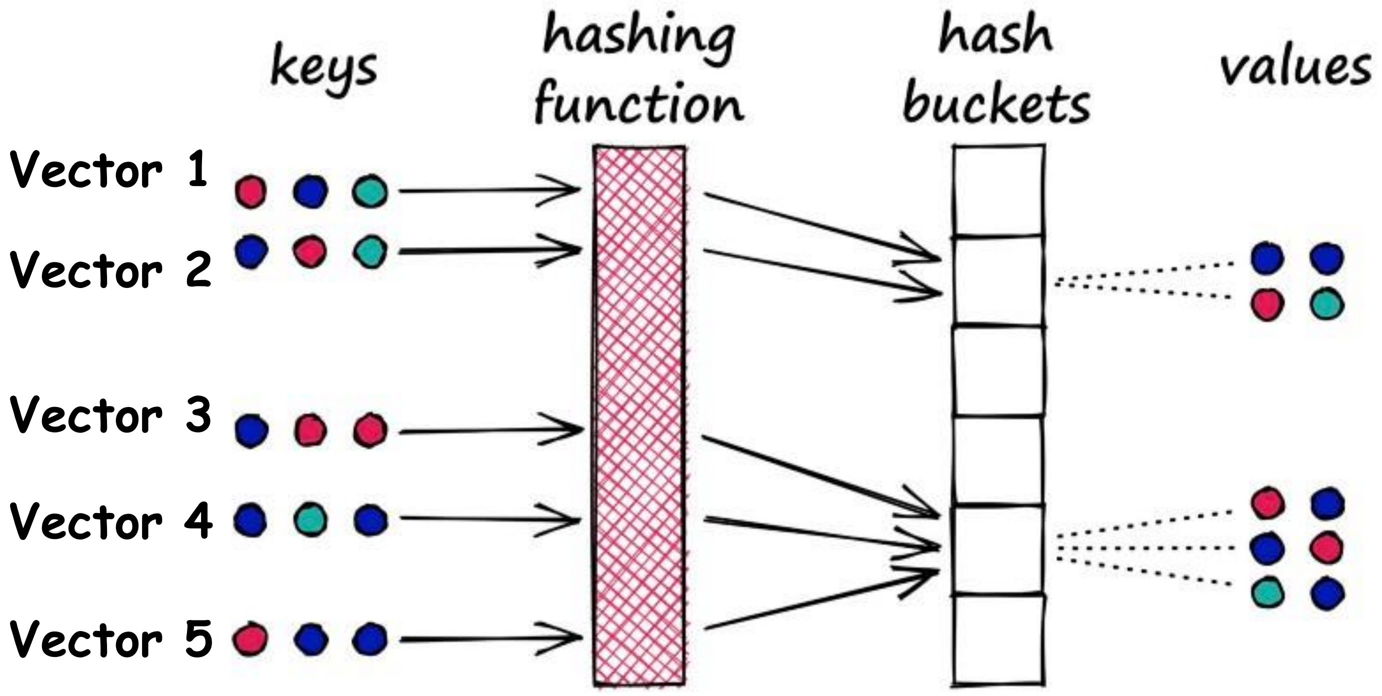
Locality Sensitive Hashing (LSH)

Instead of minimizing collisions, LSH aims at **maximizing** collisions in the sense that **similar vectors should be mapped into the same bucket**!

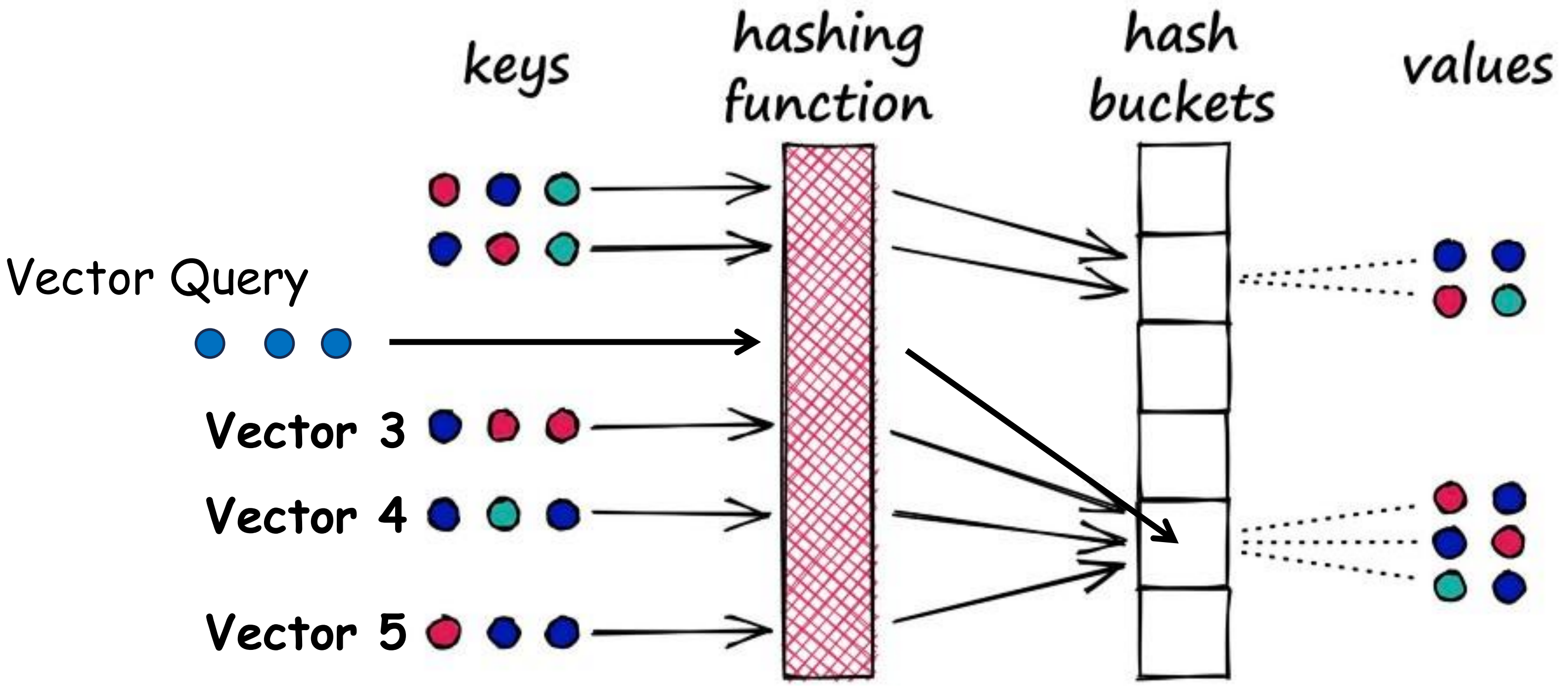


This produces groups of vectors.

https://www.pinecone.io/learn/series/faiss/vector-indexes/

Locality Sensitive Hashing (LSH)

Ketika ada **vector query**, ia akan di-hash dan akan dipetakan ke sebuah bucket. Perhitungan nearest neighbor hanya mempertimbangkan vector-vector di bucket yang sama.



Artinya, perhitungan similarity cukup dilakukan antara **Query dengan vector 3, 4, dan 5.**

https://www.pinecone.io/learn/series/faiss/vector-indexes/

How to do LSH?

One way is to perform **Random Projection** or **Random Hyperplanes**.

This is a mechanism to reduce our highly-dimensional vectors into **low-dimensionality binary vectors**.

Two similar vectors should have the same low-dimensional binary vectors --> this is our hash function that maximizes collisions!

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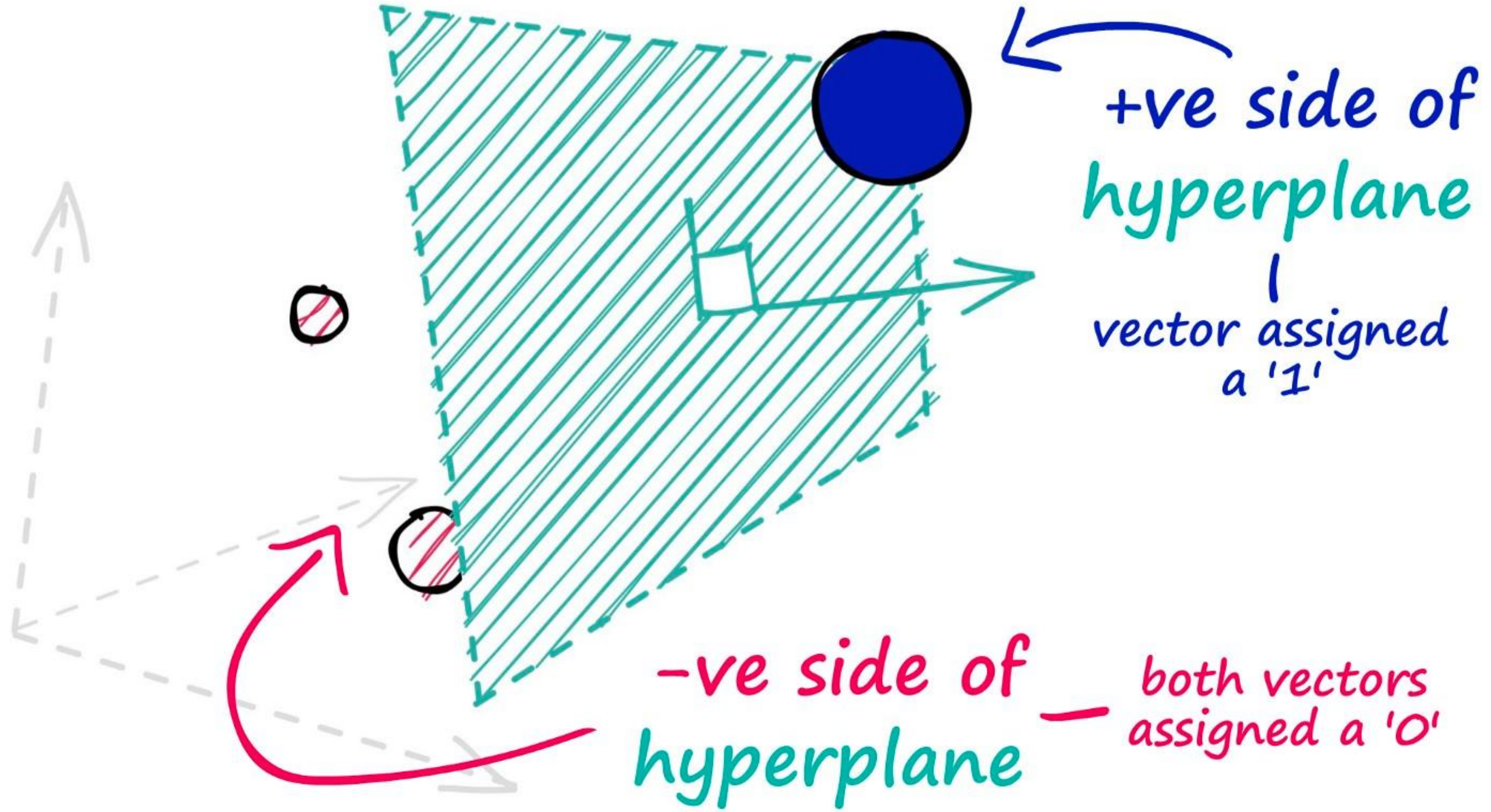
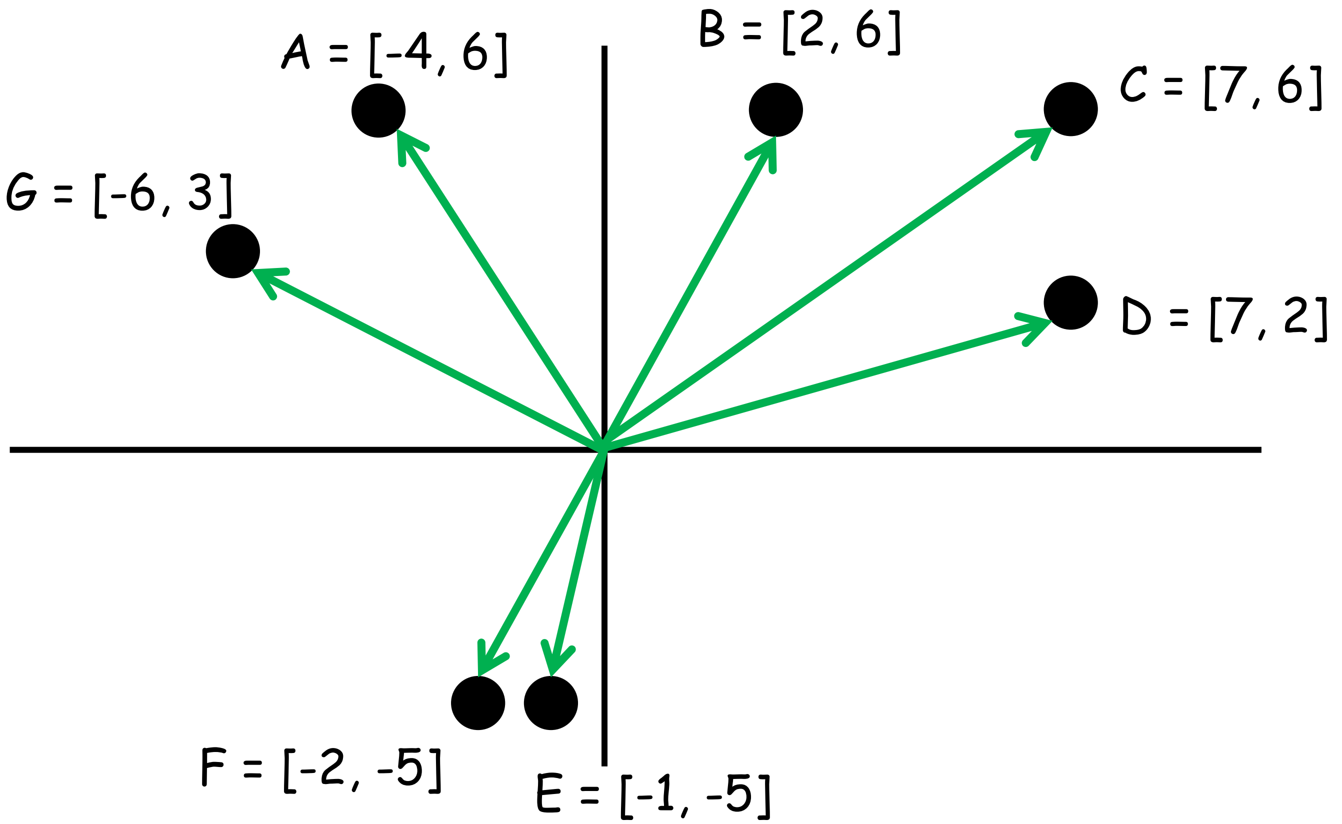
Random Projections or Hyperplanes

We assign **a value of 1** to vectors on the +ve side of our hyperplane and **a value of 0** to vectors on the -ve side of the hyperplane.



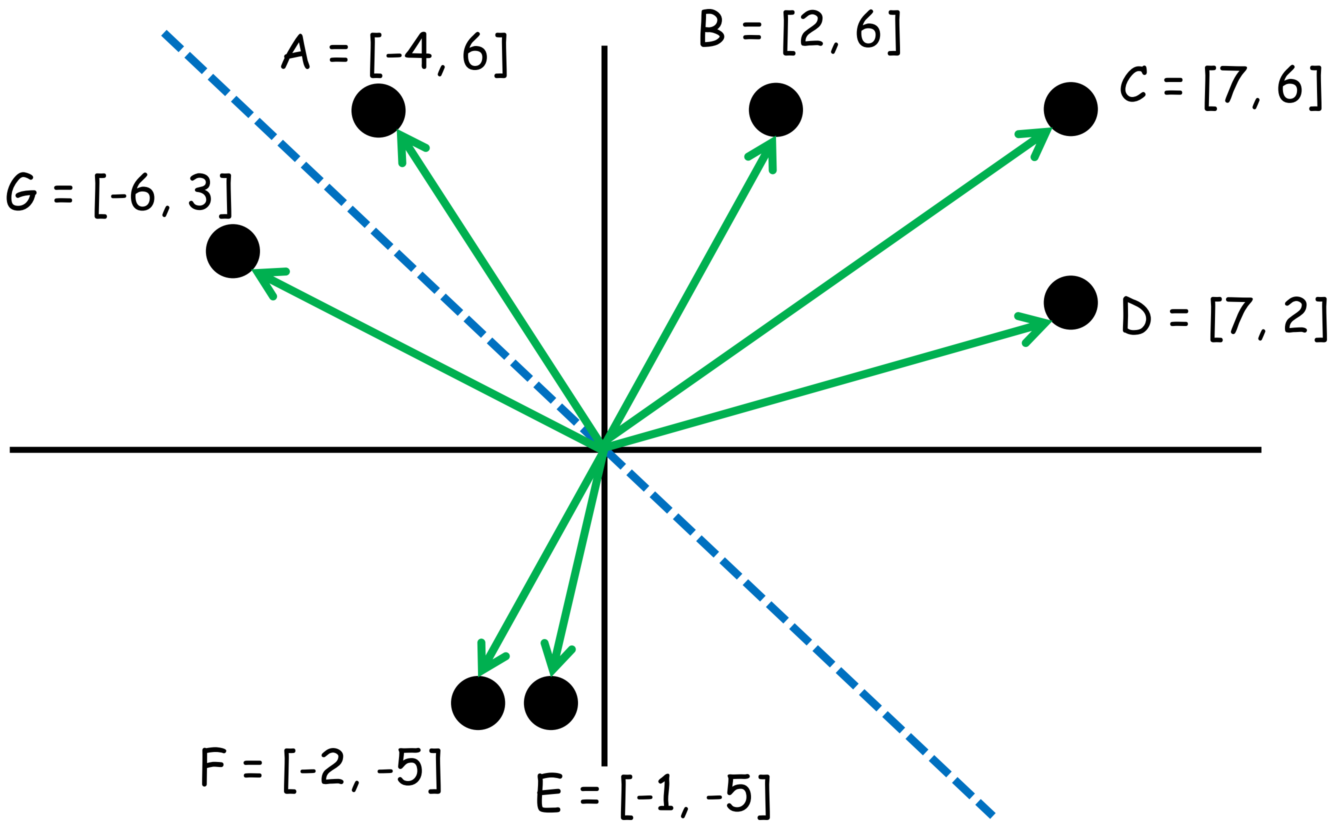
Random Projections or Hyperplanes

Misal, ada beberapa vektor 2D



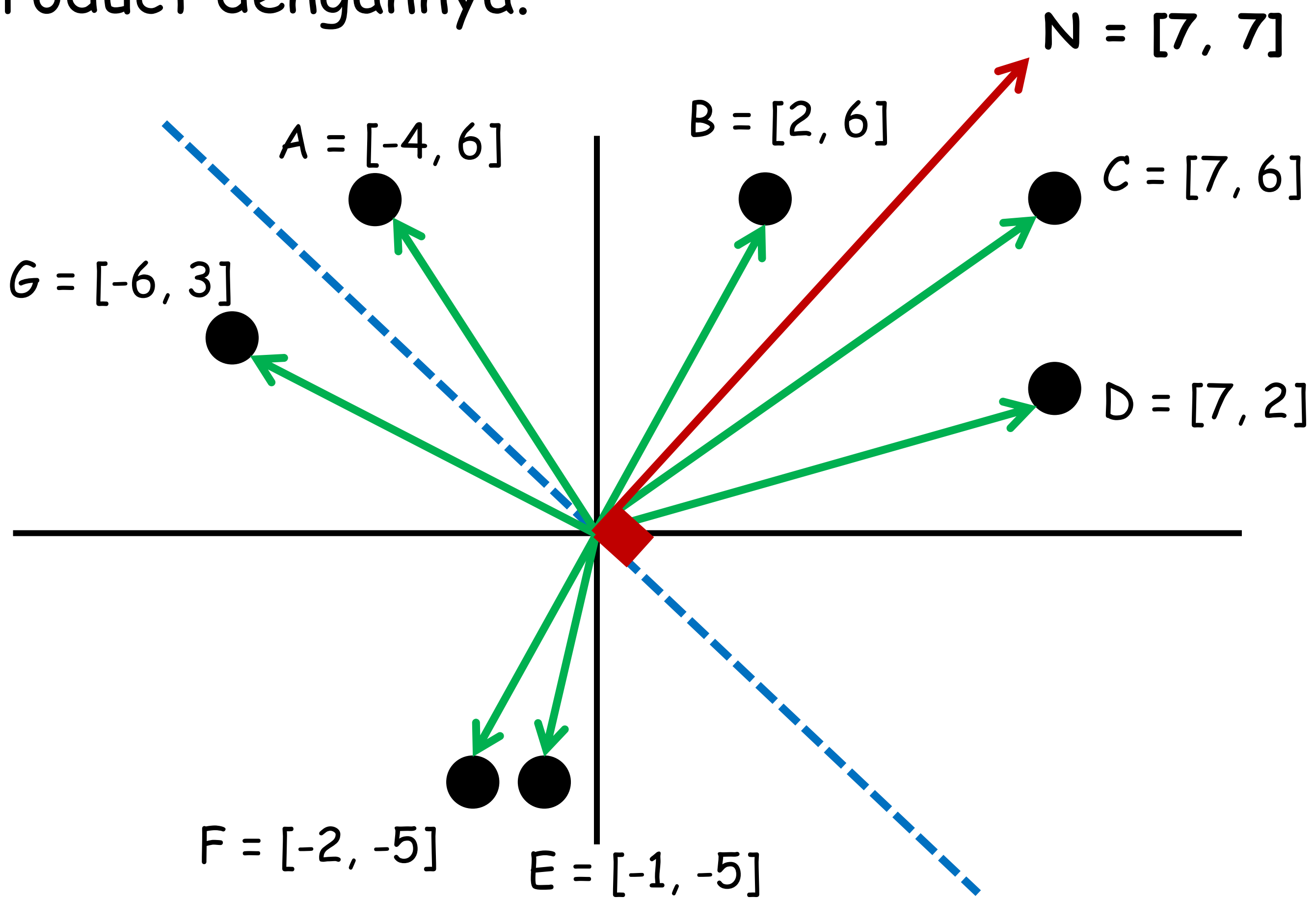
Random Projections or Hyperplanes

Misal, kita hasilkan sebuah hyperplane **secara random**!



Random Projections or Hyperplanes

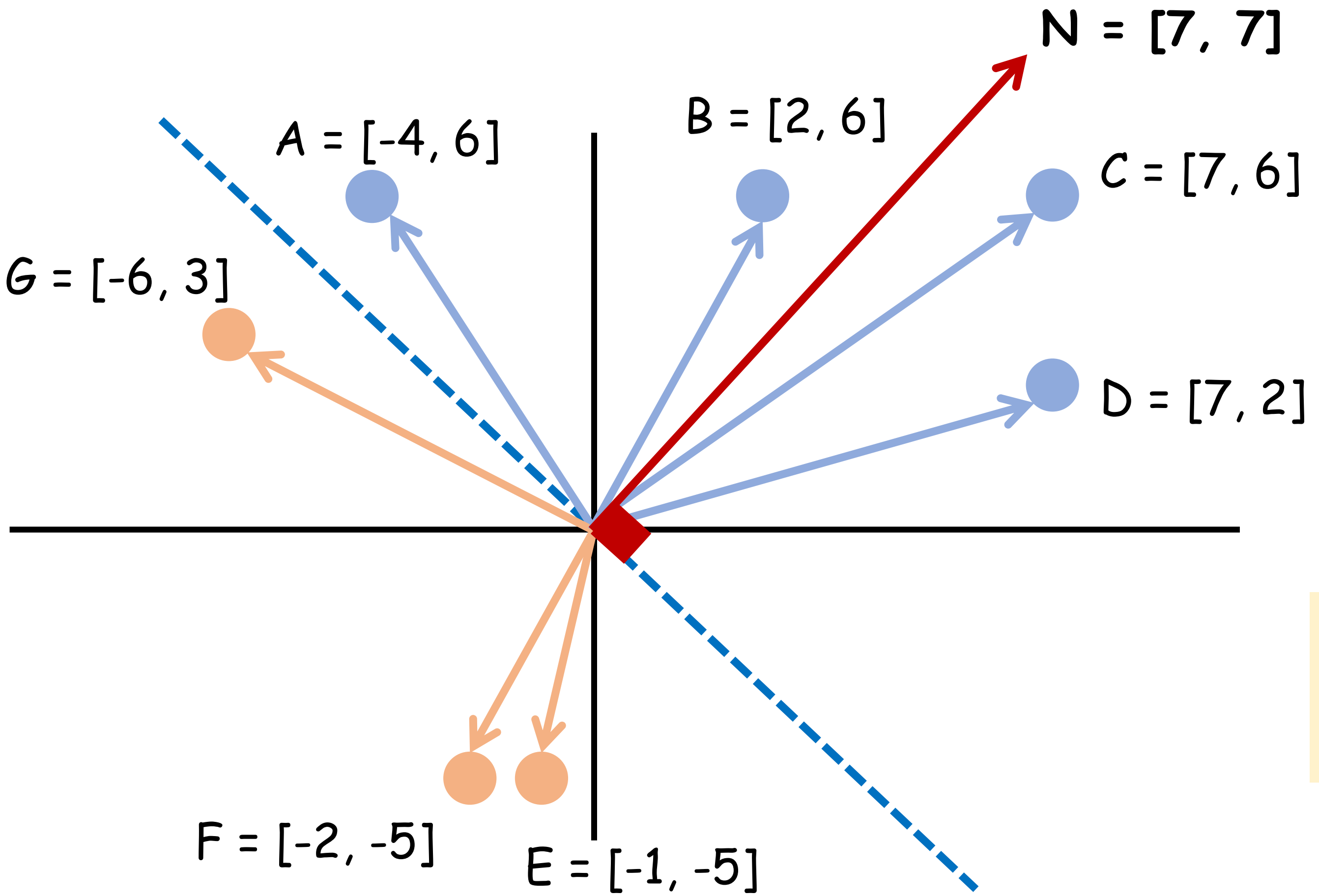
Untuk identifikasi pada sisi hyperplane mana vektor-vektor berada, kita dapat menggunakan **normal vector (tegak lurus hyperplane)**, dan melakukan dot product dengannya.



Random Projections or Hyperplanes

Jika dua vector berada pada **arah yang sama**, dot product akan menghasilkan nilai positif; dan jika tidak, dot product akan negatif.

Kita encode vektor E, F, dan G dengan **[0]**



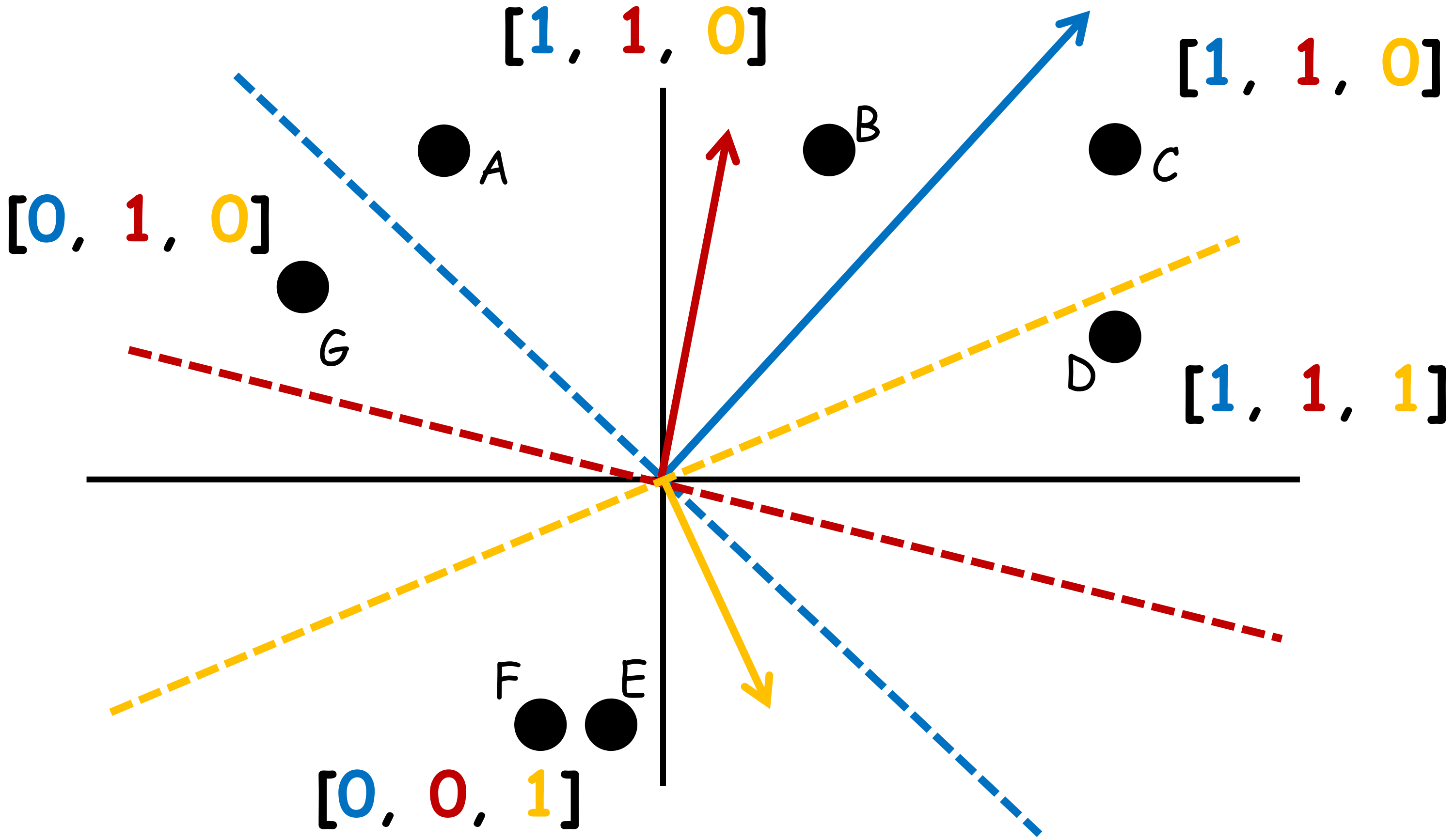
dot(A,N) > 0
dot(B,N) > 0
dot(C,N) > 0
dot(D,N) > 0

dot(G,N) < 0
dot(F,N) < 0
dot(E,N) < 0

Kita encode vektor A, B, C, dan D dengan **[1]**

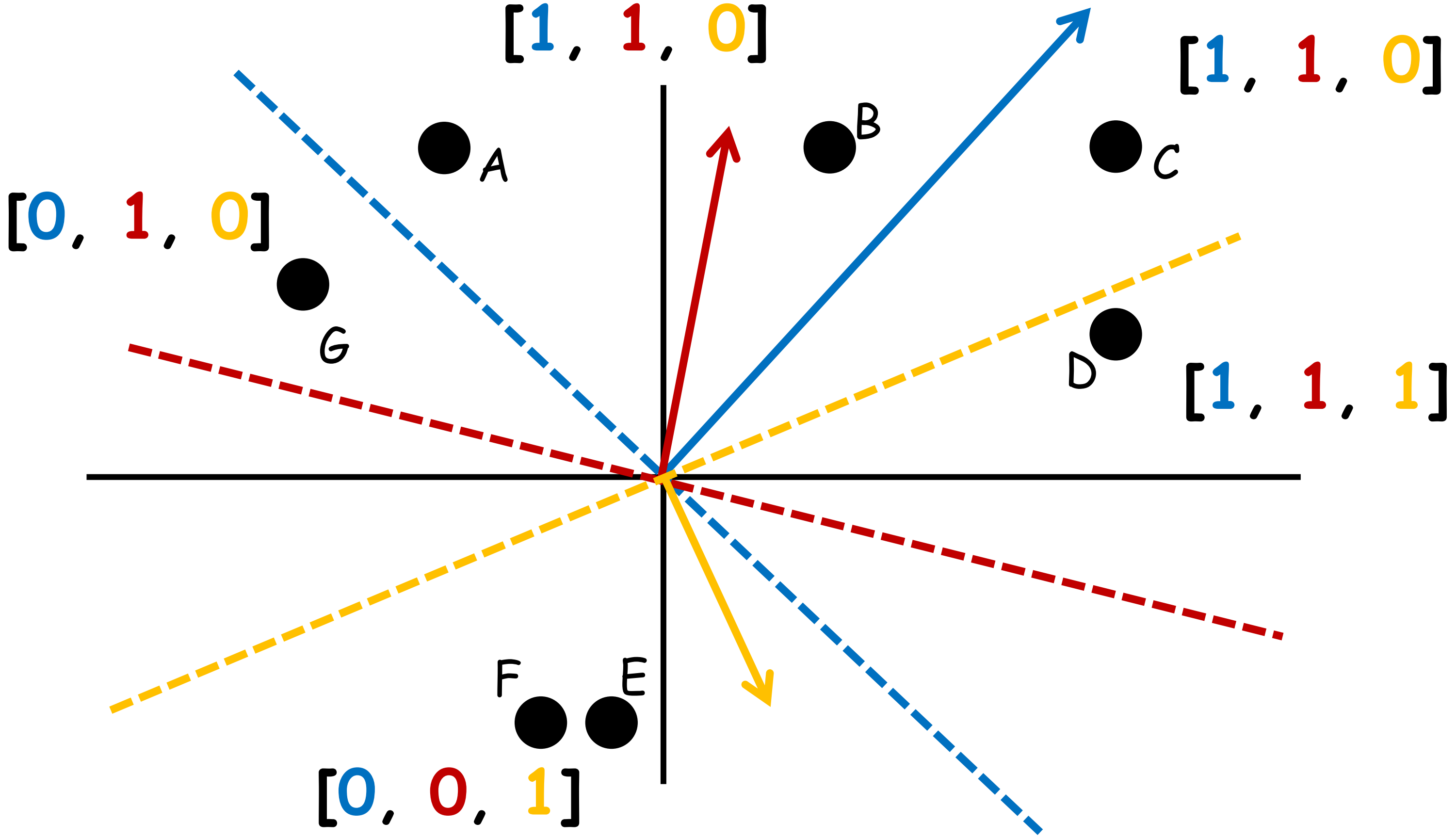
Random Projections or Hyperplanes

Kita perlu tambah **random hyperplane** agar bisa menambah informasi.
Contoh di bawah adalah dengan nbits = 3.



Random Projections or Hyperplanes

Now, we have bucketed **eight** vectors!

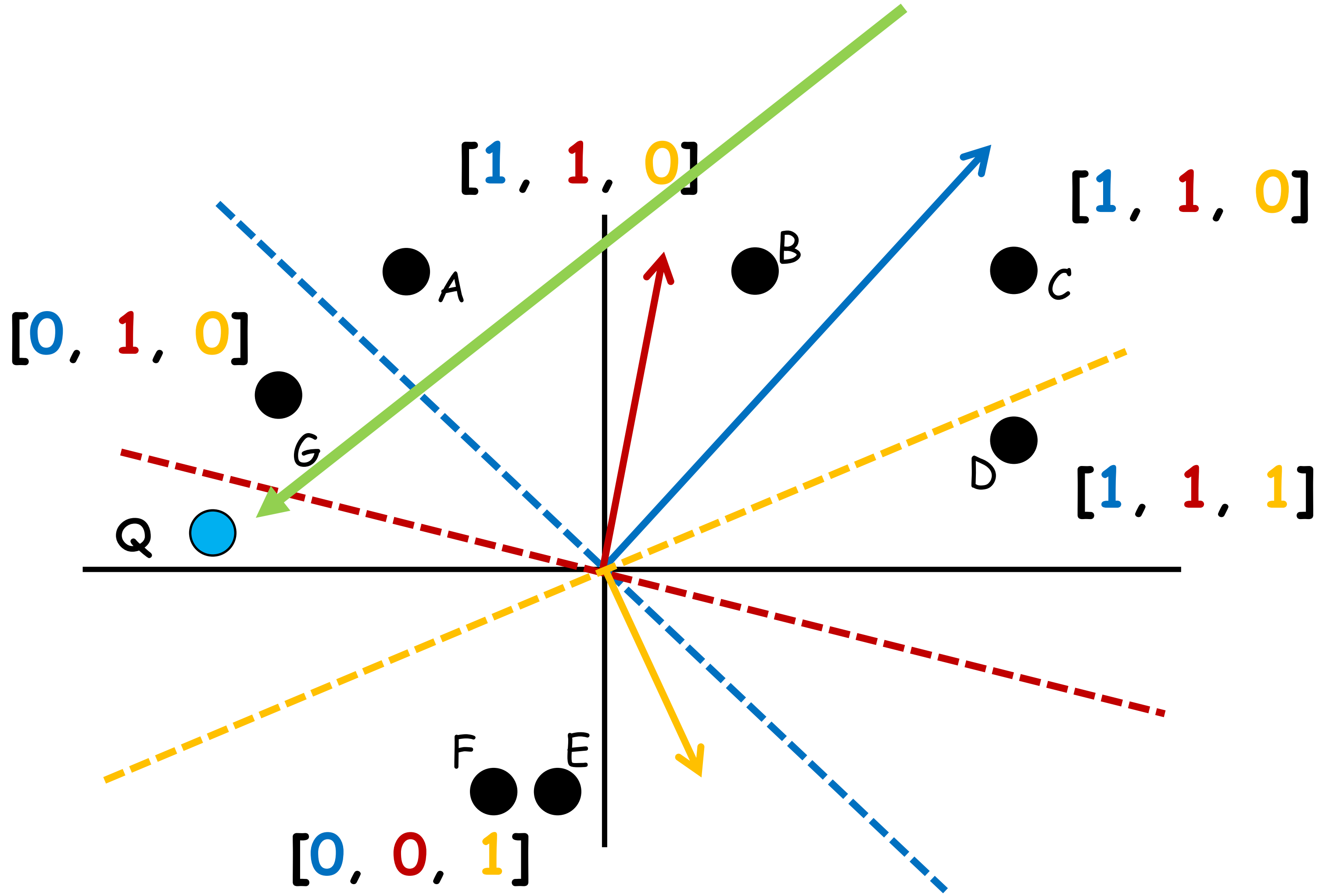



```
{'110': [A, B, C],
 '111': [D],
 '001': [E, F],
 '010': [G]}
```

This is our LSH index!

Random Projections or Hyperplanes

Misal, ada sebuah query vector **Q** yang di-hash ke [0, 0, 0]

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Random Projections or Hyperplanes

Misal, ada sebuah query vector **Q** yang di-hash ke **[0, 0, 0]**

Kita kemudian bandingkan query vector **Q** dengan semua **bucket** pada LSH index kita; dan ambil **Top-K vectors**.

Kita bisa gunakan **Hamming Distance**, yang menghitung "mismatch" antara dua binary vectors.

```
{'110': [A, B, C],
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```

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Random Projections or Hyperplanes

Misal, ada sebuah query vector **Q** yang di-hash ke **[0, 0, 0]**

Hamming Distance

```
def hamming_distance(string1, string2) :

  if len(string1) != len(string2):
    raise ValueError("Panjang string harus sama.")

  num_mismatch = 0
  for n in range(len(string1)):
    if string1[n] != string2[n]:
      num_mismatch += 1
  return num_mismatch
```

```
{'110': [A, B, C],
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```

This is our LSH index!

Random Projections or Hyperplanes

Misal, ada sebuah query vector **Q** yang di-hash ke **[**0, 0, 0**]**

Hamming Distance (HD), misal **K = 3**

HD('000', '110') = 2

HD('000', '111') = 3

HD('000', '001') = 1

HD('000', '010') = 1

```
{'110': [A, B, C],
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 '001': [E, F],
 '010': [G]}
```

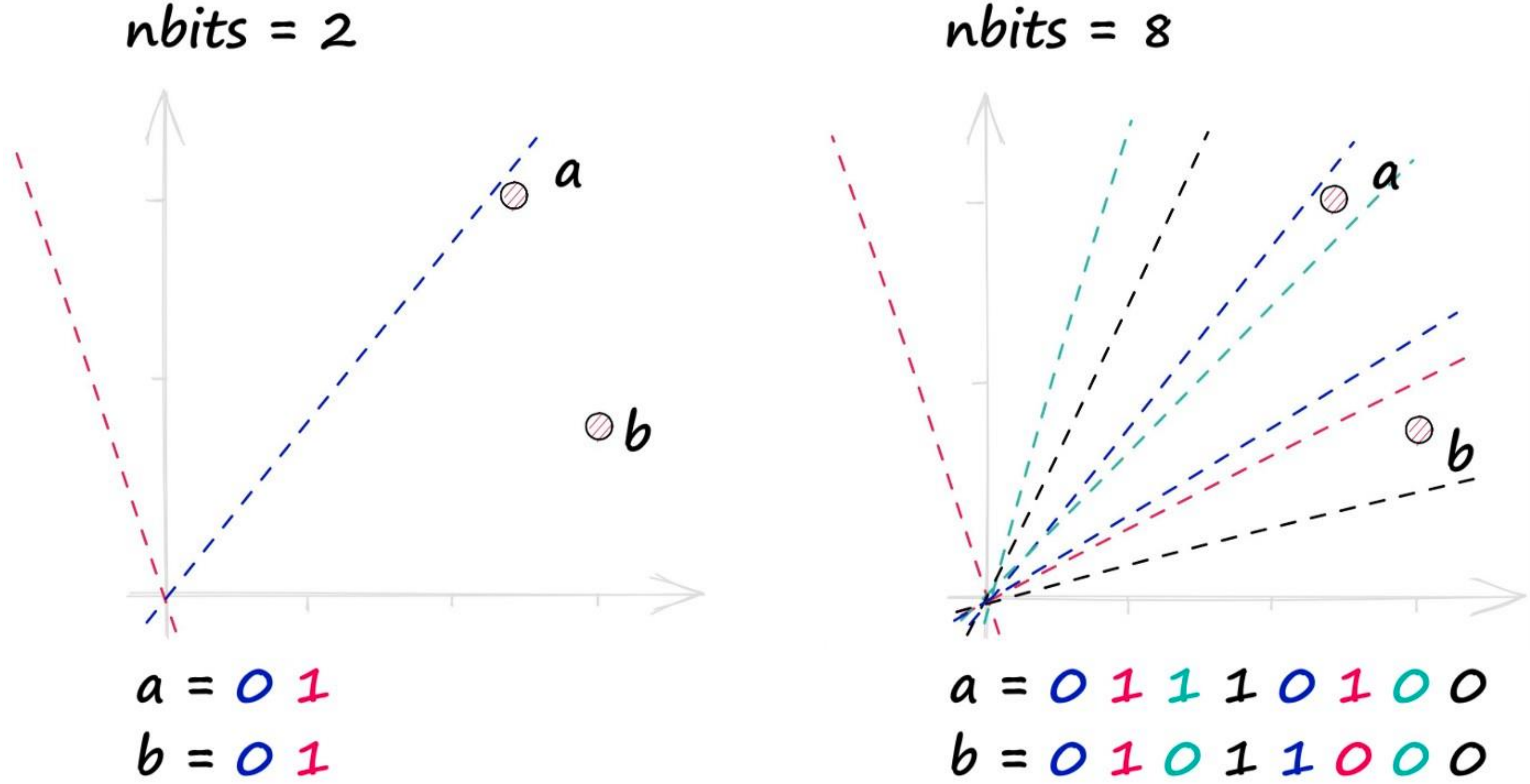
This is our LSH index!

Top-3 = [E, F, G]

* Kita juga bisa re-ranking 3 top vectors ini berdasarkan nilai Cosine Similarity dengan Q

In reality, we use many more hyperplanes — more hyperplanes mean higher resolution binary vectors — producing much more precise representations of our vectors.

A higher **nbits** value improves search quality by increasing the resolution of hashed vectors.



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Contoh Implementasi (Toy Implementation)

https://github.com/pinecone-io/examples/blob/master/learn/search/faiss-ebook/locality-sensitive-hashing-random-projection/random_projection.ipynb

```python
def all_binary(n):
    total = 1 << n
    print(f"{total} possible combinations")
    combinations = []
    for i in range(total):
        # get binary representation of integer
        b = bin(i)[2:]
        # pad zeros to start of binary representtion
        b = '0' * (n - len(b)) + b
        b = [int(i) for i in b]
        combinations.append(b)
    return combinations
```

https://github.com/pinecone-io/examples/blob/master/learn/search/faiss-ebook/locality-sensitive-hashing-random-projection/random_projection.ipynb

```python
class RandomProjection:
    # initialize what will be the buckets
    buckets = {}
    # initialize counter
    counter = 0

    def __init__(self, nbits, d):
        self.nbits = nbits
        self.d = d
        # create our hyperplane normal vecs for splitting data
        self.plane_norms = np.random.rand(d, nbits) - .5
        print(f"Initialized {self.plane_norms.shape[1]} hyperplane normal vectors.")
        # add every possible combination to hashes attribute as numpy array
        self.hashes = all_binary(nbits)
        # and add each as a key to the buckets dictionary
        for hash_code in self.hashes:
            # convert to string
            hash_code = ''.join([str(i) for i in hash_code])
            self.buckets[hash_code] = []
        # convert self.hashes to numpy array
        self.hashes = np.stack(self.hashes)
```

https://github.com/pinecone-io/examples/blob/master/learn/search/faiss-ebook/locality-sensitive-hashing-random-projection/random_projection.ipynb

```python
def get_binary(self, vec):
    # calculate nbits dot product values
    direction = np.dot(vec, projection.plane_norms)
    # find positive direction (>0) and negative direction (<=0)
    direction = direction > 0
    # convert boolean array to integer strings
    binary_hash = direction.astype(int)
    return binary_hash

def hash_vec(self, vec, show=False):
    # generate hash
    binary_hash = self.get_binary(vec)
    # convert to string format for dictionary
    binary_hash = ''.join(binary_hash.astype(str))
    # add ID to buckets dictionary
    self.buckets[binary_hash].append(self.counter)
    if show:
        print(f"{self.counter}: {''.join(binary_hash)}")
    # increment counter
    self.counter += 1
```

https://github.com/pinecone-io/examples/blob/master/learn/search/fais-ebook/locality-sensitive-hashing-random-projection/random_projection.ipynb

```python
def hamming(self, hashed_vec):
    # get hamming distance between query vec and all buckets in self.hashes
    hamming_dist = \
        np.count_nonzero(hashed_vec != projection.hashes, axis=1).reshape(-1, 1)
    # add hash values to each row
    hamming_dist = np.concatenate((projection.hashes, hamming_dist), axis=1)
    # sort based on distance
    hamming_dist = hamming_dist[hamming_dist[:, -1].argsort()]
    return hamming_dist
```

https://github.com/pinecone-io/examples/blob/master/learn/search/faiss-ebook/locality-sensitive-hashing-random-projection/random_projection.ipynb

```python
def top_k(self, vec, k=5):
    # generate hash
    binary_hash = self.get_binary(vec)
    # calculate hamming distance between all vectors
    hamming_dist = self.hamming(binary_hash)
    # loop through each bucket until we have k or more vector IDs
    vec_ids = []
    for row in hamming_dist:
        str_hash = ''.join(row[:-1].astype(str))
        bucket_ids = self.buckets[str_hash]
        vec_ids.extend(bucket_ids)
        if len(vec_ids) >= k:
            vec_ids = vec_ids[:k]
            break
    # return top k IDs
    return vec_ids
```

https://github.com/pinecone-io/examples/blob/master/learn/search/faiss-ebook/locality-sensitive-hashing-random-projection/random_projection.ipynb

Hierarchical Navigable Small Worlds

Semua materi diambil tanpa malu dari:

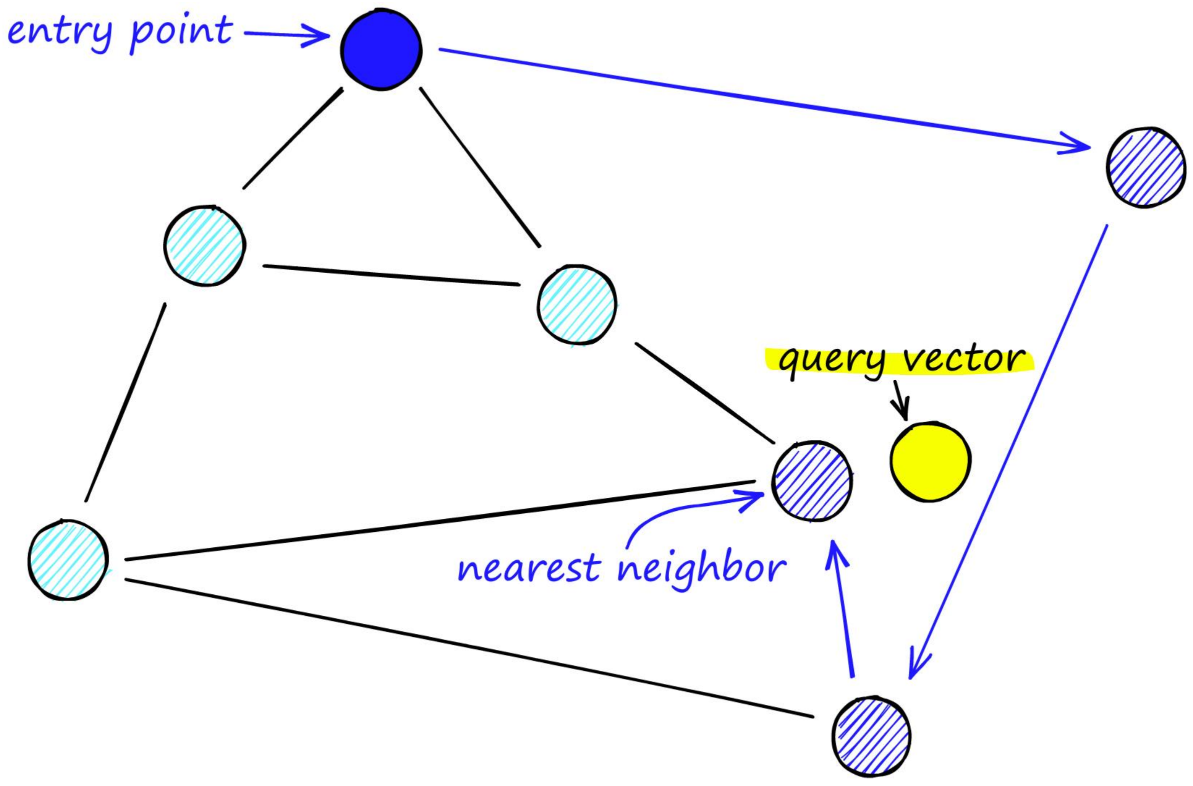
https://www.pinecone.io/learn/series/faiss/hnsw/

https://towardsdatascience.com/similarity-search-part-4-hierarchical-navigable-small-world-hnsw-2aad4fe87d37

Navigable Small World Graphs

When searching an NSW graph, we begin at a pre-defined ***entry-point***. This entry point connects to several nearby vertices. We identify which of these vertices is the closest to our query vector and move there.

We repeat the **greedy-routing search** process of moving from vertex to vertex by identifying the nearest neighboring vertices in each friend list. **Eventually, we will find no nearer vertices than our current vertex** — this is a local minimum and acts as our **stopping condition**.



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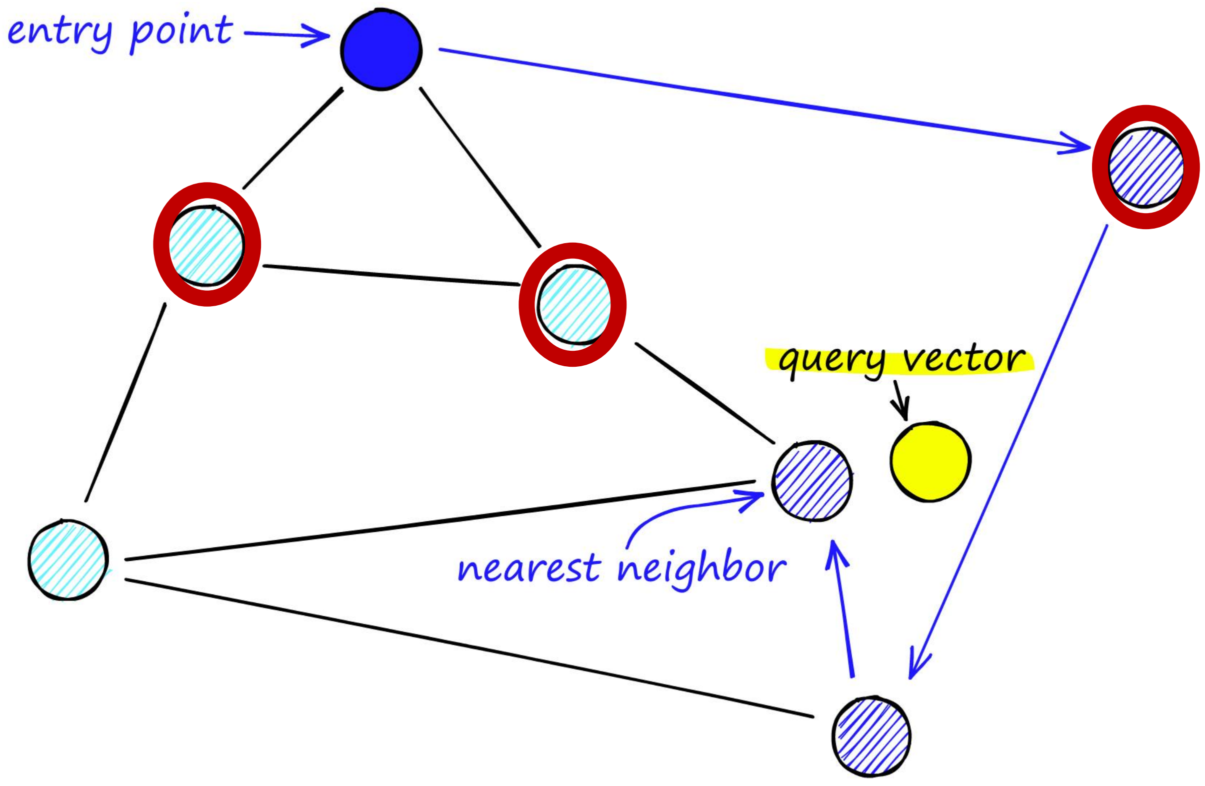

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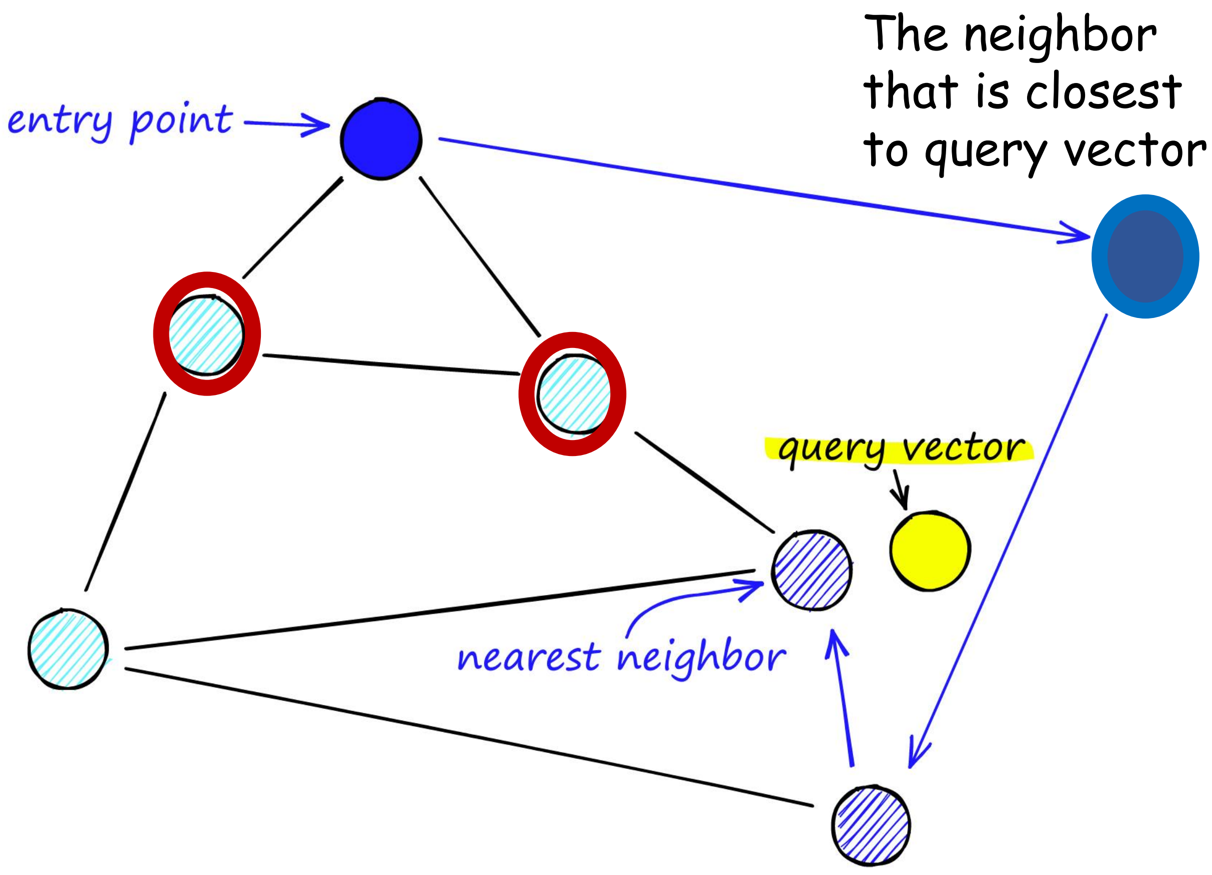

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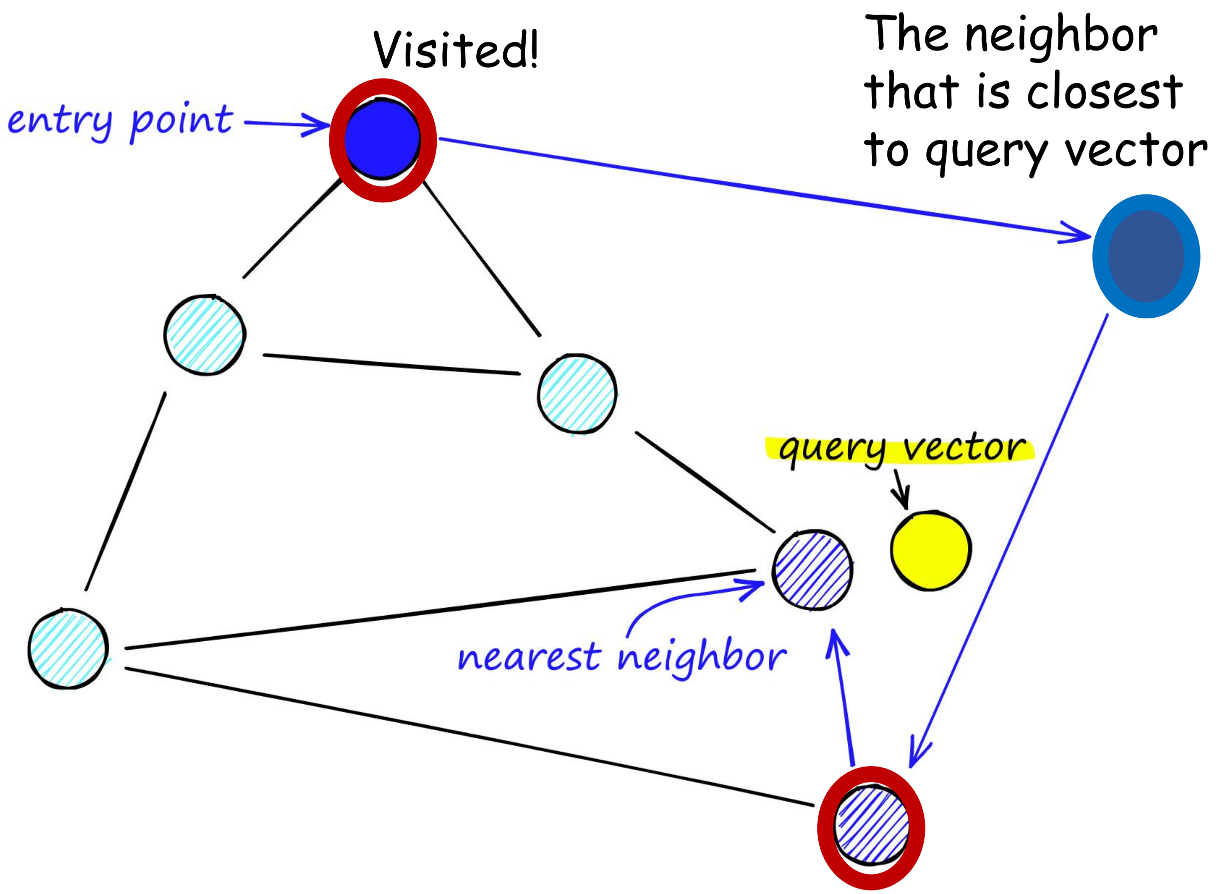

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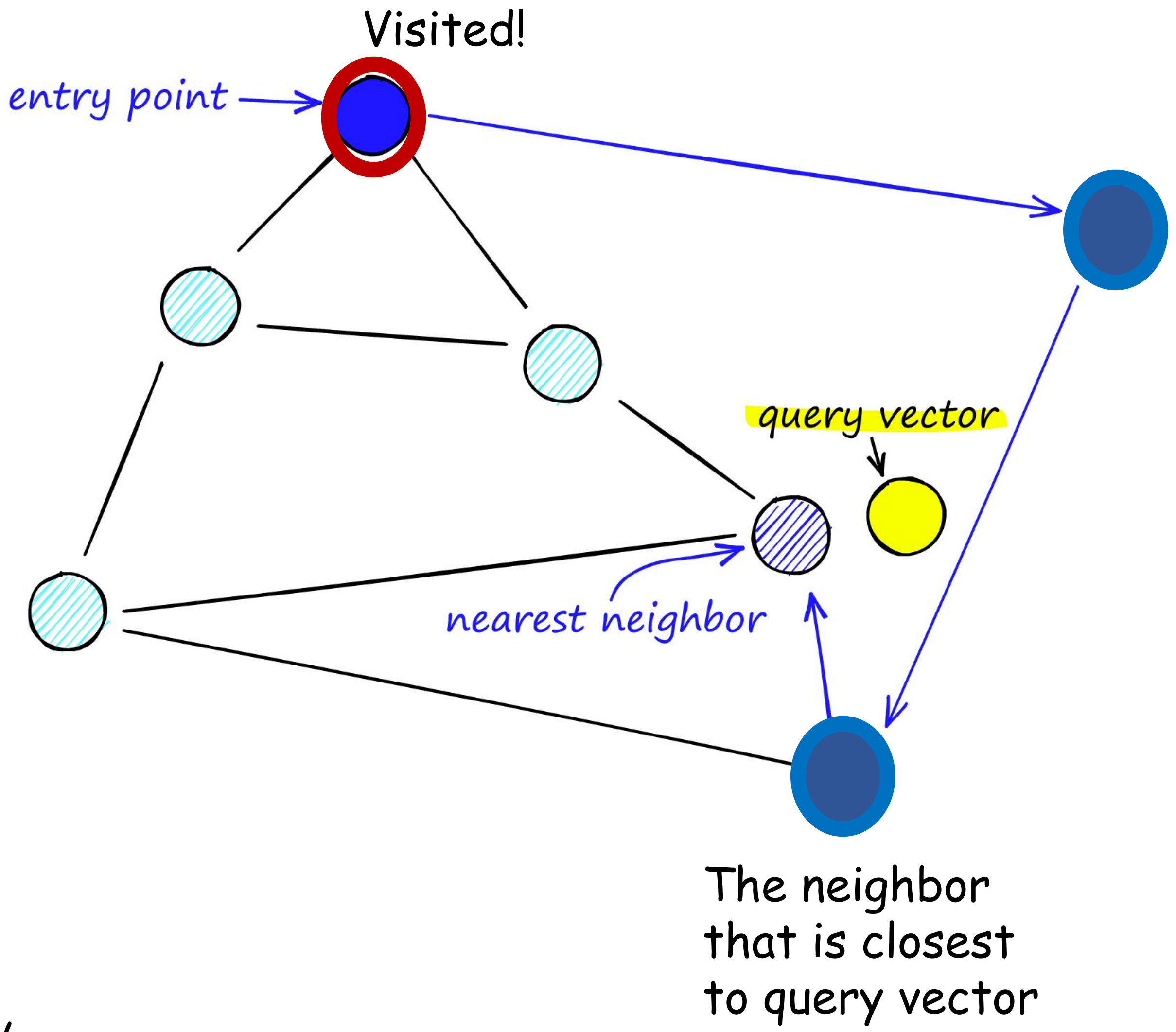

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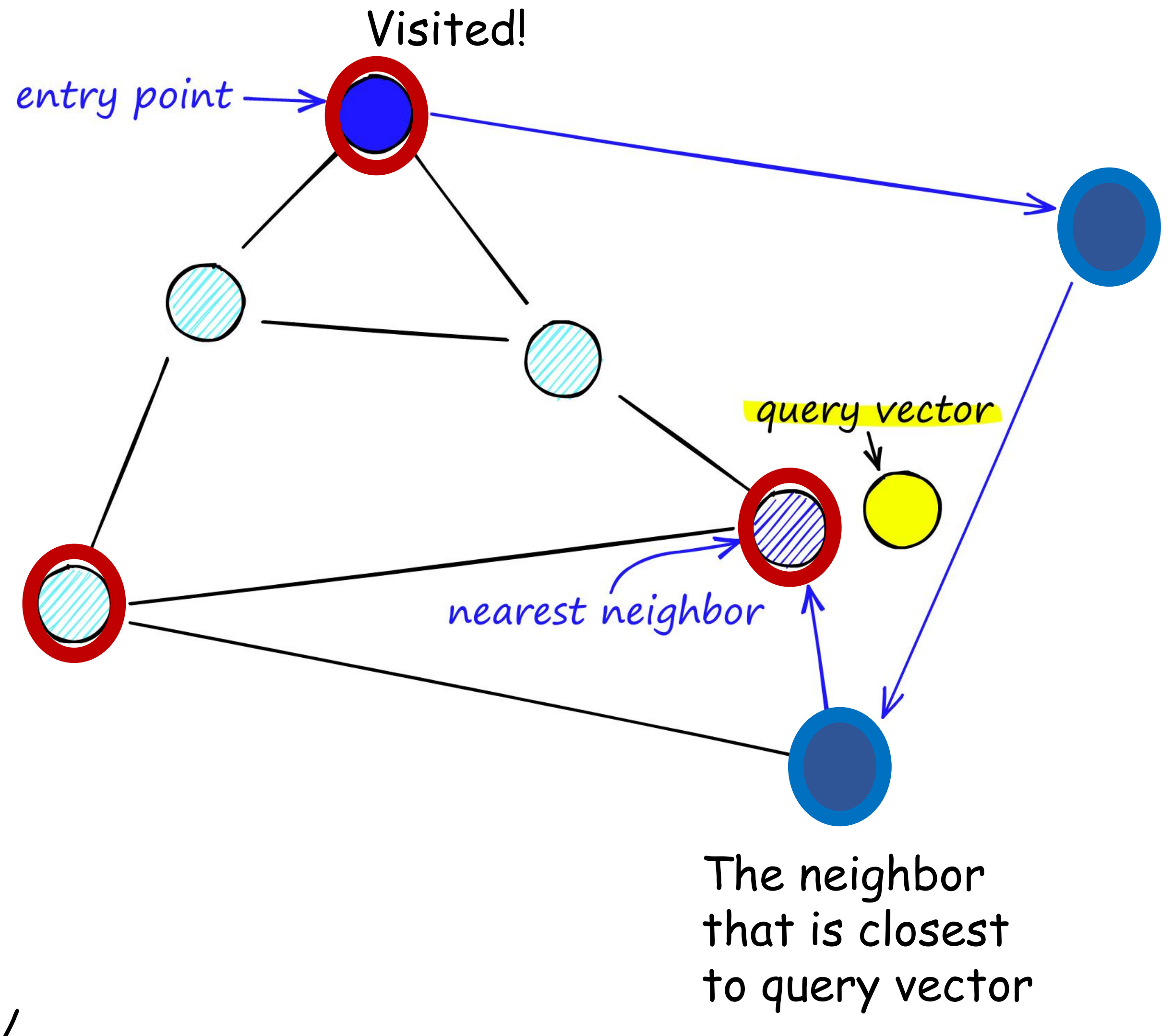

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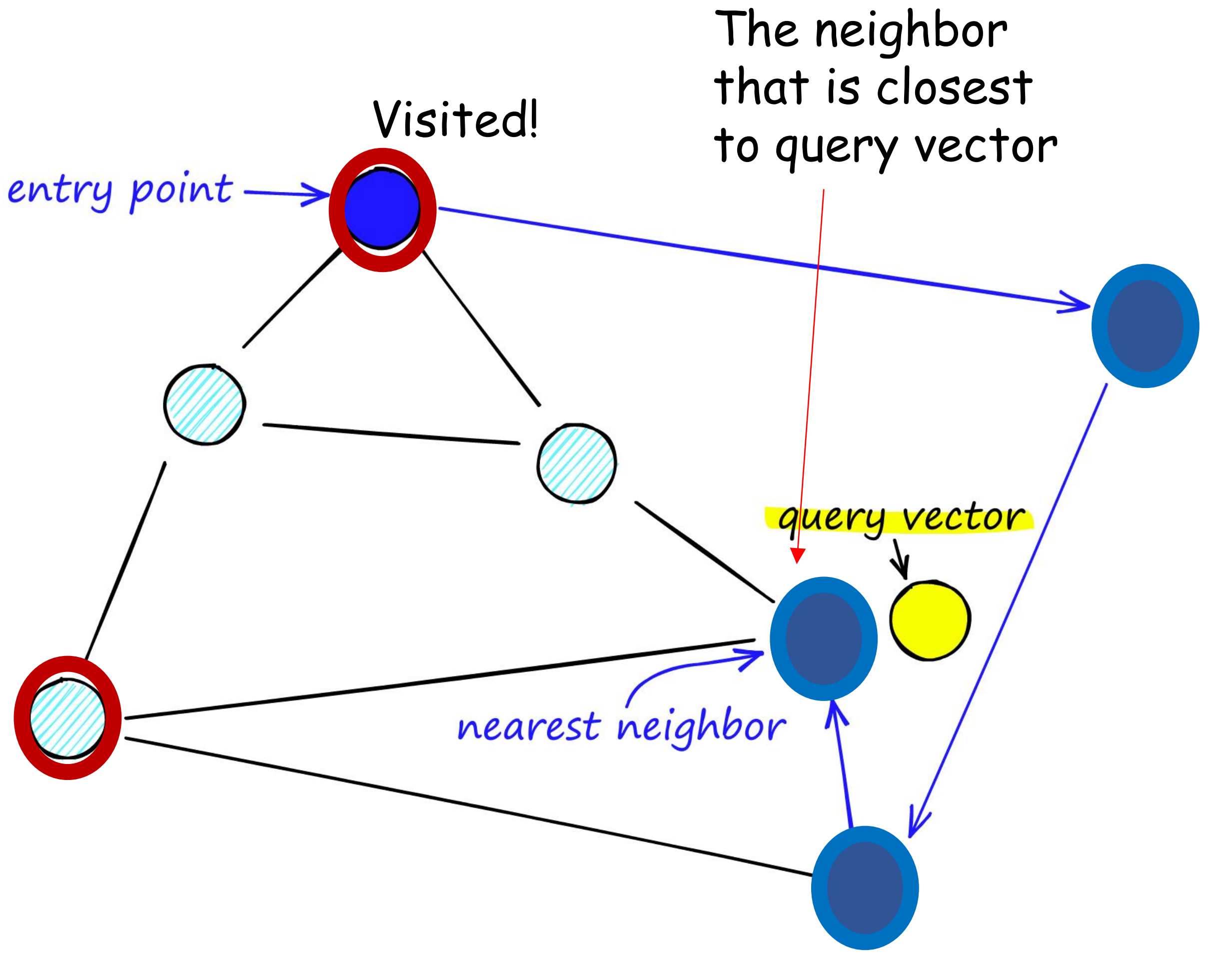

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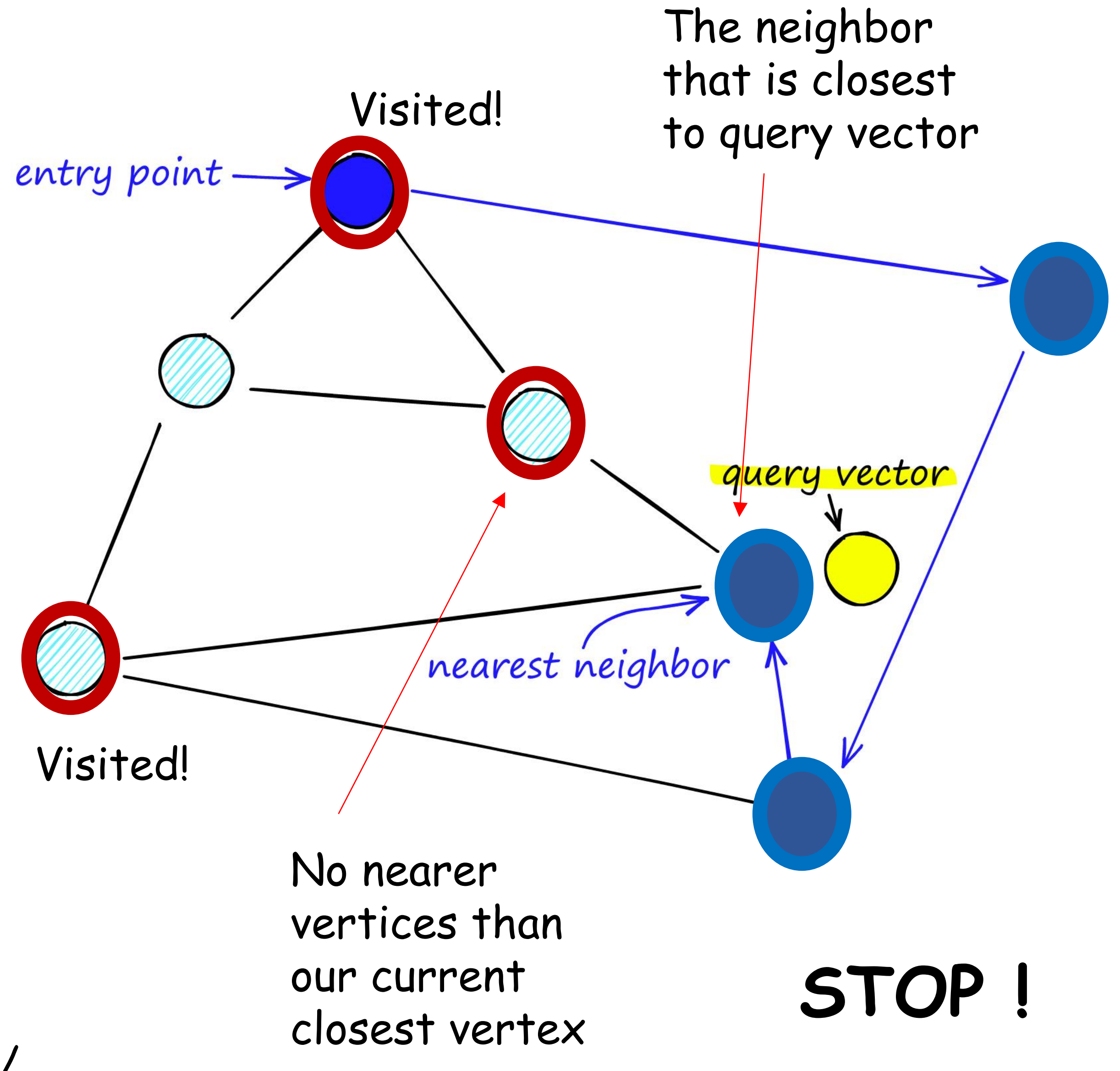

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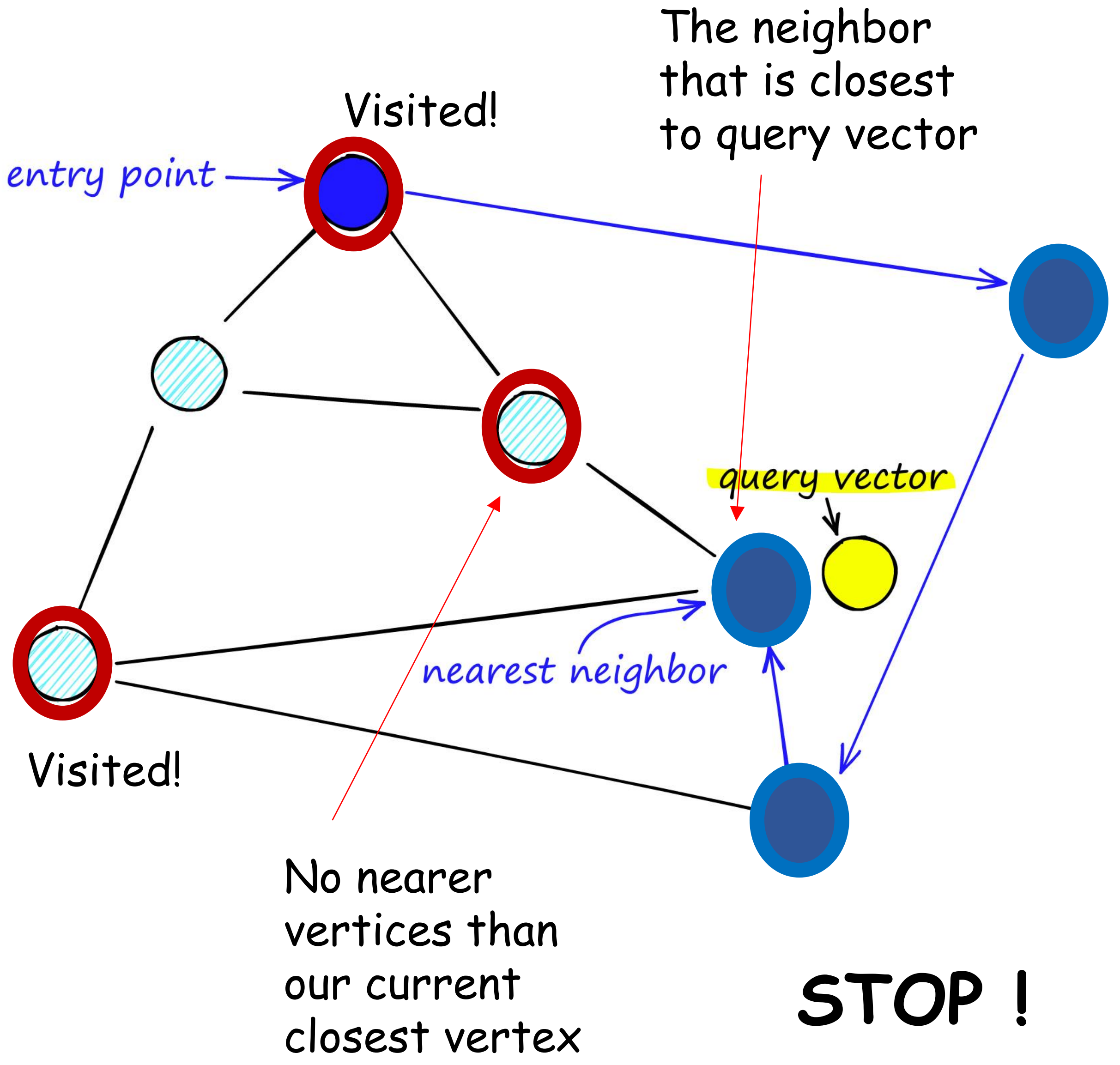
Navigable Small World Graphs

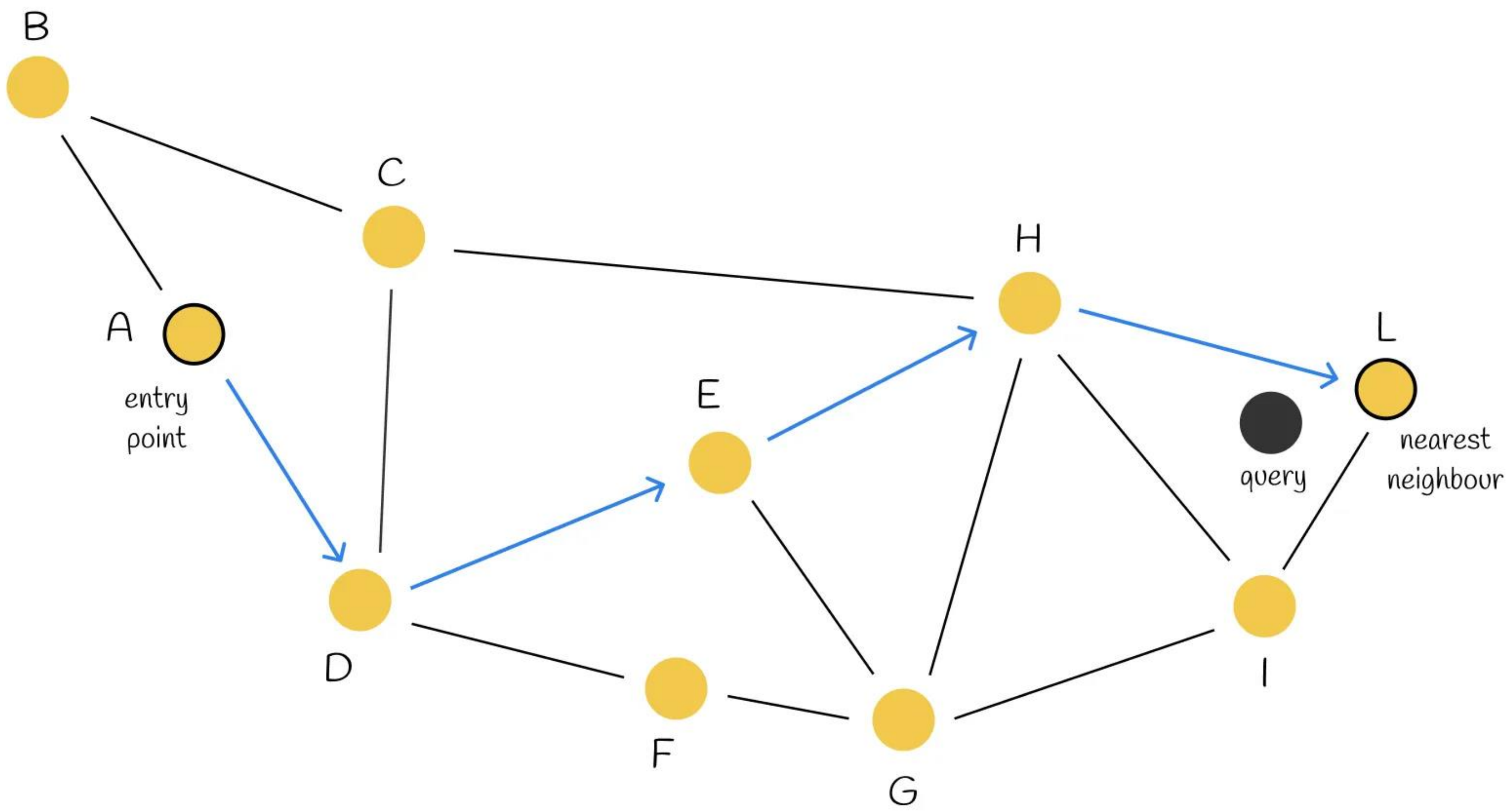
Secara praktis, proses seperti ini dilakukan secara berulang-ulang untuk mendapatkan **K buah nearest vectors**.

Setiap run, kita "entry point" bisa diacak.



Navigable Small World Graphs

Contoh lain:



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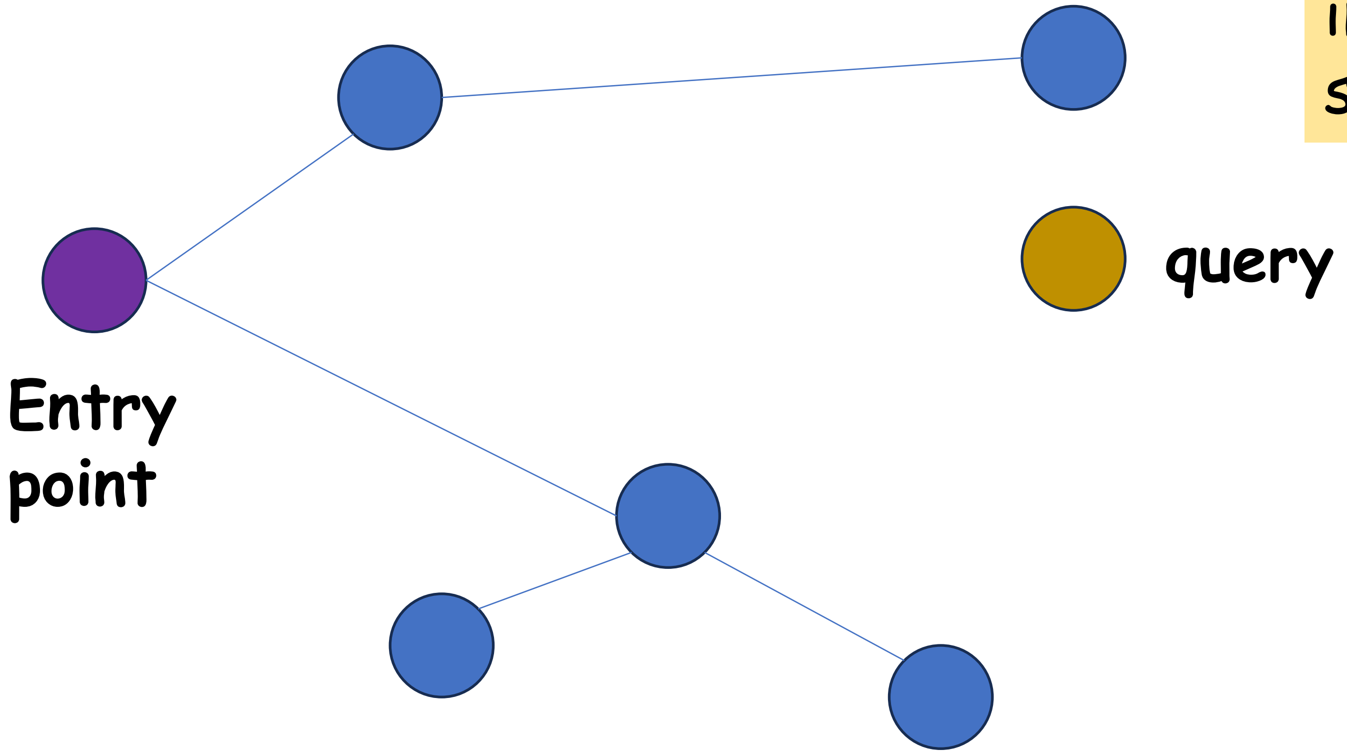
Navigable Small World Graphs



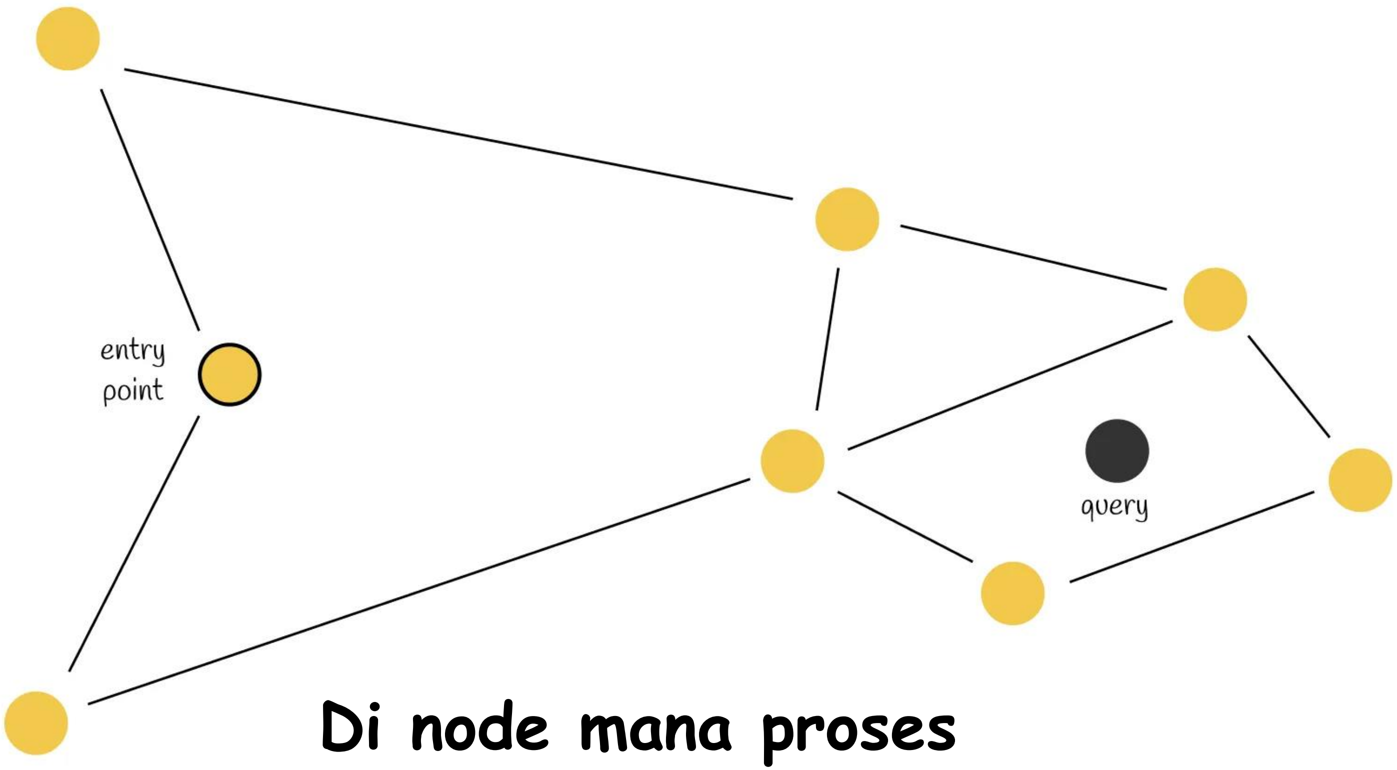
This greedy strategy **does not guarantee** that it will find the exact nearest neighbor as the method uses only local information at the current step to take decisions.

Navigable Small World Graphs

Problem:

Early stopping is one of the problems of the algorithm.

For the most part, this might happen when the starting region has too many **low-degree vertices**.



Di node mana proses search akan berhenti?

https://towardsdatascience.com/similarity-search-part-4-hierarchical-navigable-small-world-hnsw-2aad4fe87d37

Indexing
(Constructing Navigable Small World Graphs)

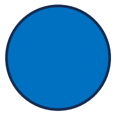
How to construct NSW? (indexing)

- **Sebuah node = sebuah vektor**
- **Node A dekat dengan Node B = vektor A dan vektor B "similar" (cosine sim., Euclidean dist., dsb.)**

- Misal, **M** adalah banyaknya tetangga terdekat untuk node yang baru "masuk".
- Pada setiap iterasi, sebuah node baru ditambahkan ke dalam index dan dihubungkan dengan **M** buah tetangga terdekat.

Constructing Navigable Small World Graphs

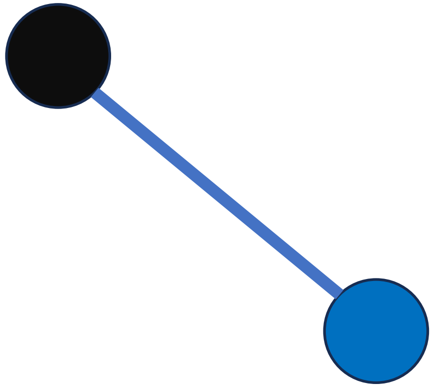
M = 2



Node biru: vektor yang baru dimasukkan ke index
Sisi biru: sisi yang baru terbentuk

Constructing Navigable Small World Graphs

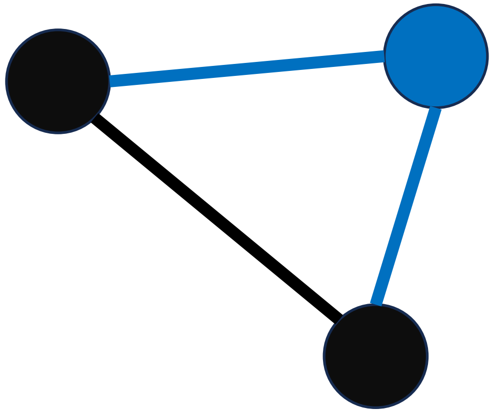
M = 2



Node biru: vektor yang baru dimasukkan ke index
Sisi biru: sisi yang baru terbentuk

Constructing Navigable Small World Graphs

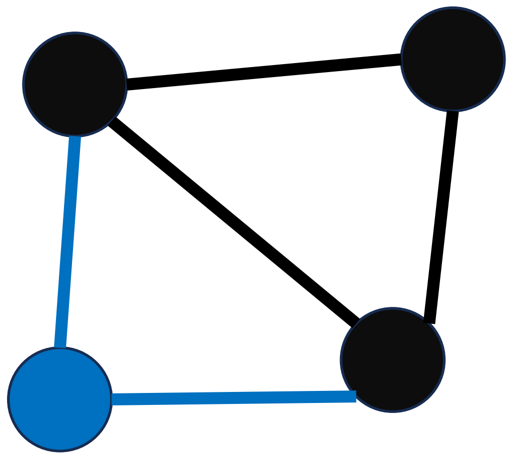
M = 2



Node biru: vektor yang baru dimasukkan ke index
Sisi biru: sisi yang baru terbentuk

Constructing Navigable Small World Graphs

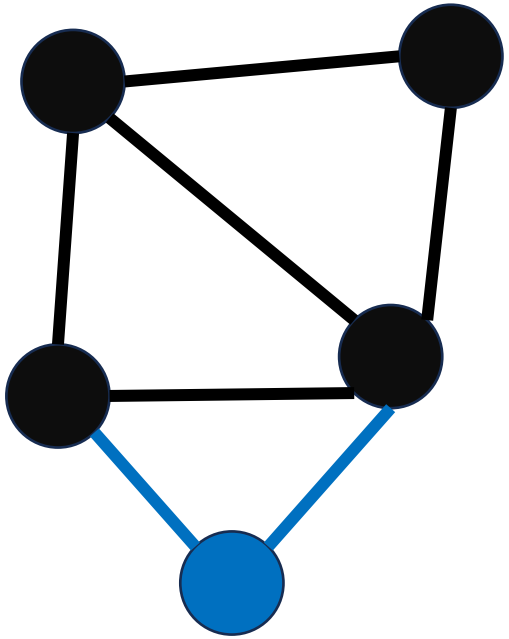
M = 2



Node biru: vektor yang baru dimasukkan ke index
Sisi biru: sisi yang baru terbentuk

Constructing Navigable Small World Graphs

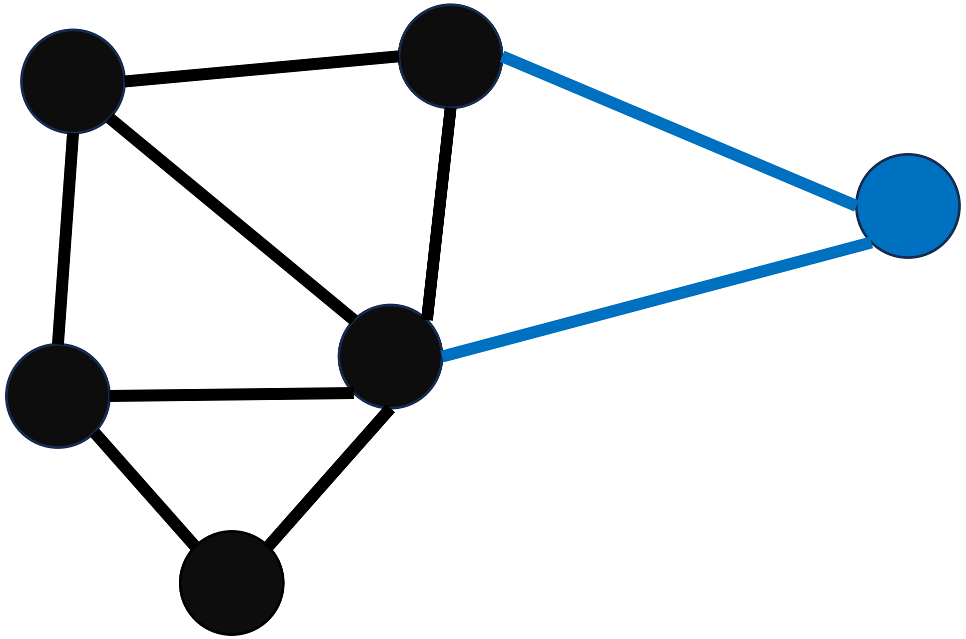
M = 2



Node biru: vektor yang baru dimasukkan ke index
Sisi biru: sisi yang baru terbentuk

Constructing Navigable Small World Graphs

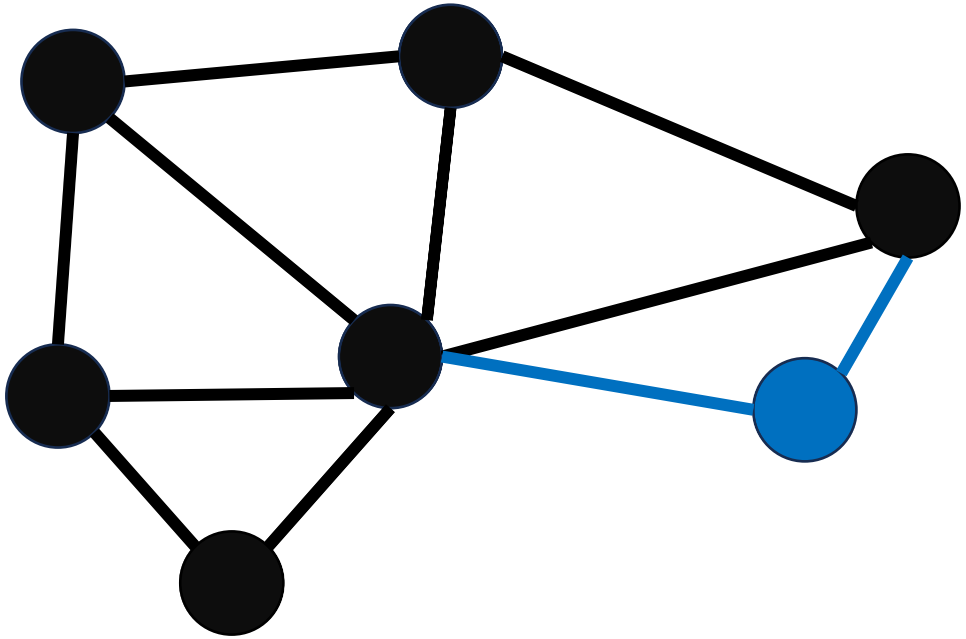
M = 2



Node biru: vektor yang baru dimasukkan ke index
Sisi biru: sisi yang baru terbentuk

Constructing Navigable Small World Graphs

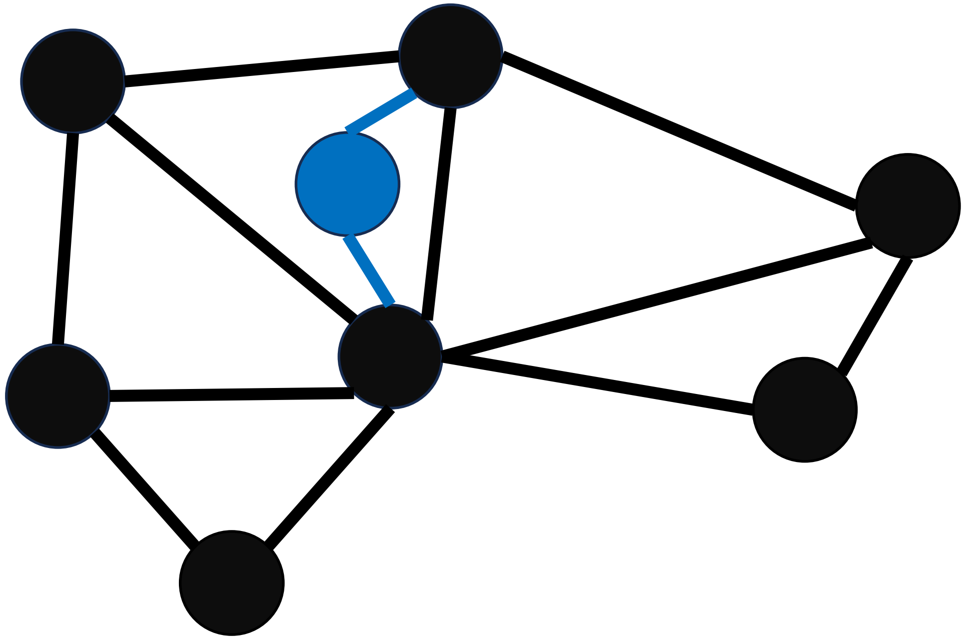
M = 2



Node biru: vektor yang baru dimasukkan ke index
Sisi biru: sisi yang baru terbentuk

Constructing Navigable Small World Graphs

M = 2



Node biru: vektor yang baru dimasukkan ke index
Sisi biru: sisi yang baru terbentuk

Make them “Hierarchical”

Hierarchical NSW = HNSW

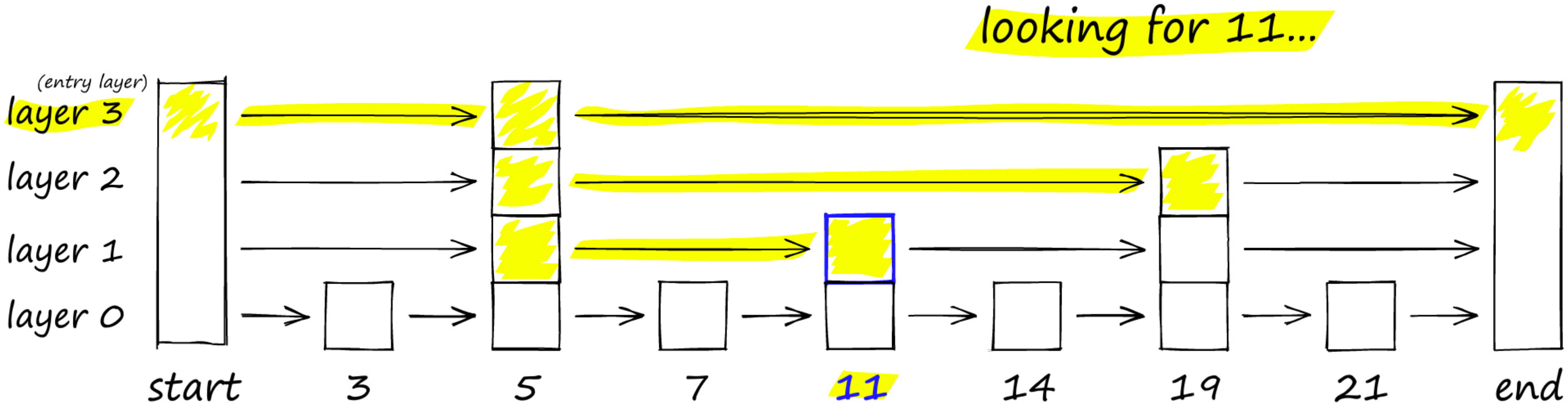
Efficient and robust approximate nearest neighbor search using Hierarchical Navigable Small World graphs

Yu. A. Malkov, D. A. Yashunin

Abstract — We present a new approach for the approximate K-nearest neighbor search based on navigable small world graphs with controllable hierarchy (Hierarchical NSW, HNSW). The proposed solution is fully graph-based, without any need for additional search structures, which are typically used at the coarse search stage of the most proximity graph techniques. Hierarchical NSW incrementally builds a multi-layer structure consisting from hierarchical set of proximity graphs (layers) for nested subsets of the stored elements. The maximum layer in which an element is present is selected randomly with an

https://www.pinecone.io/learn/series/faiss/hnsw/

Probability Skip List - Fast Search



To search a skip list, we start at the highest layer with the longest *'skips'* and move along the edges towards the right (below). If we find that the current node 'key' is *greater than* the key we are searching for — we know we have overshot our target, so we move down to previous node in the *next* level.

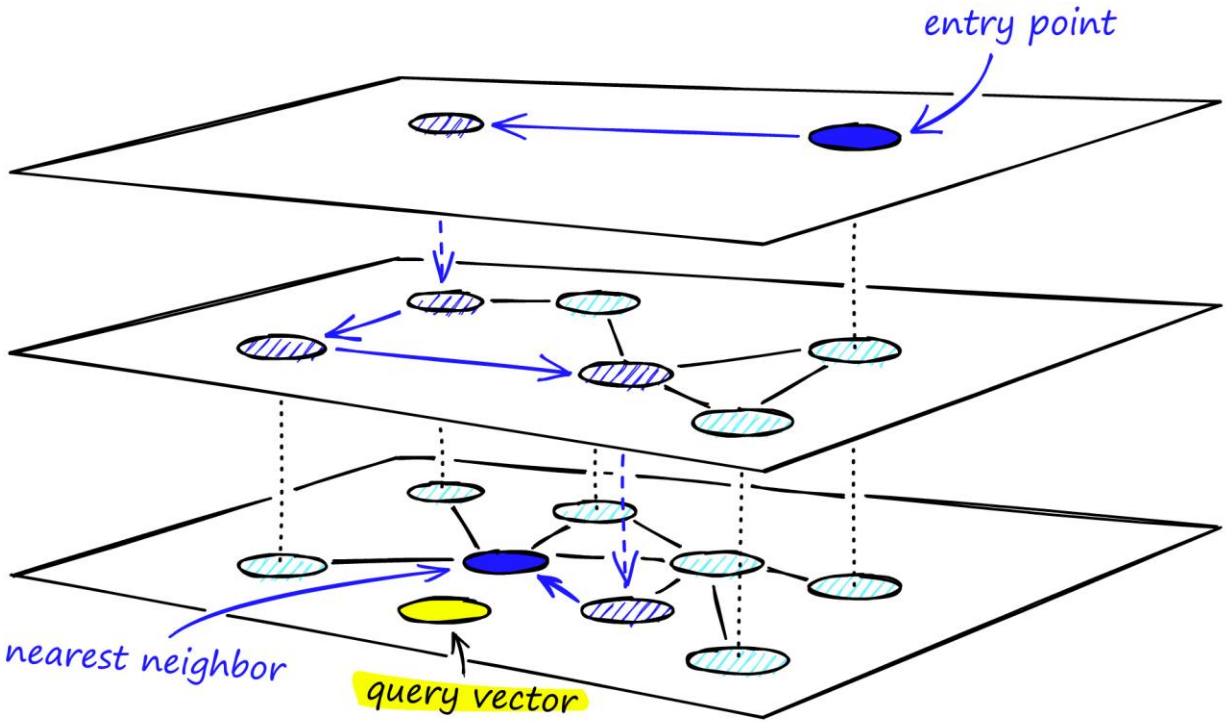
A skip list has the main parameter ***p*** which defines **the probability of an element appearing in several lists**. If an element appears in **layer *i***, then the probability that it will appear in **layer *i* + *1*** is equal to ***p***.

Insert & search: **On average O(Log N)**

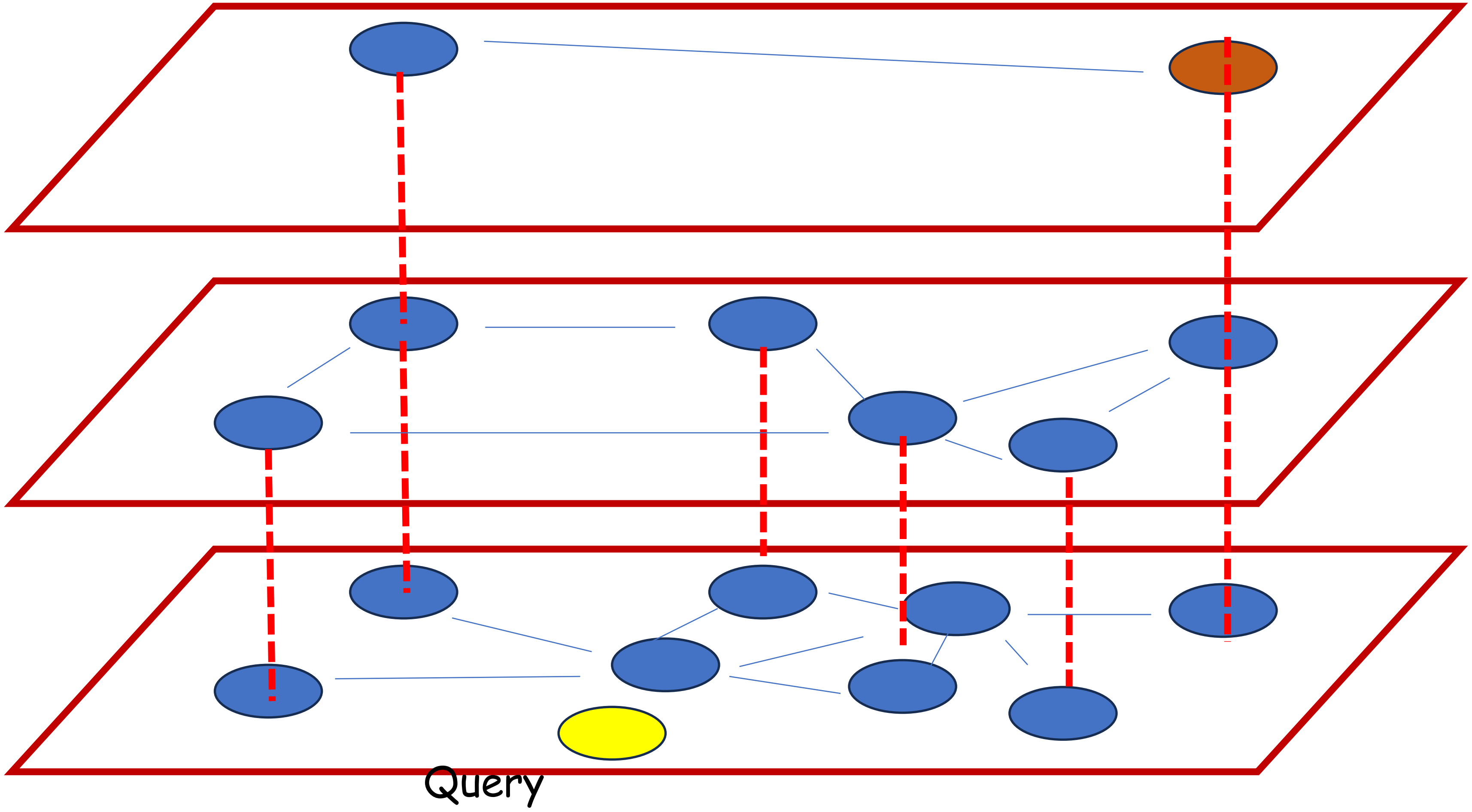
Hierarchical Navigable Small World Graphs

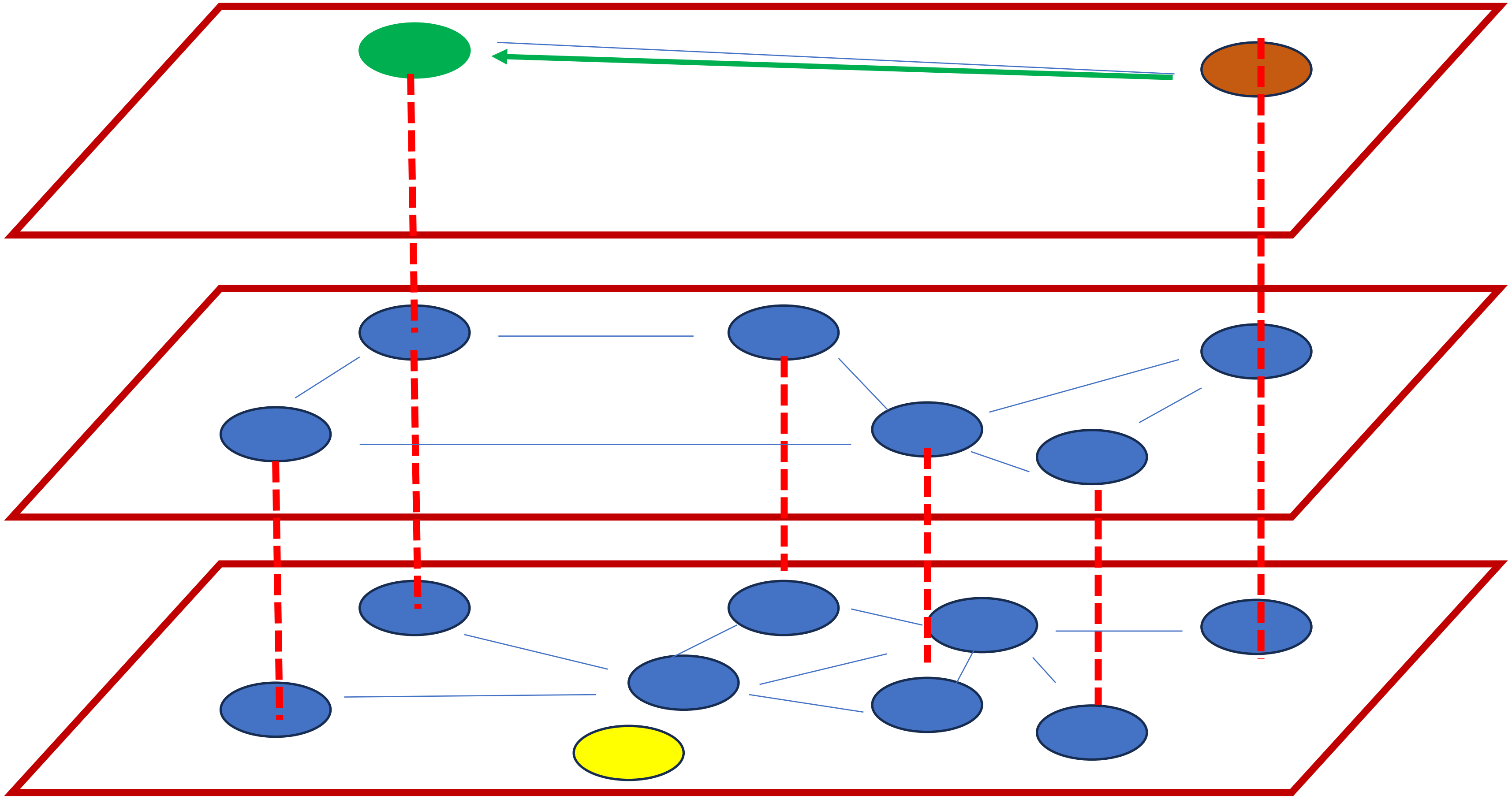
During the search, we enter the top layer. These vertices will tend to be **higher-degree vertices** (with links separated across multiple layers), meaning that we, by default, start in the **zoom-in phase.**

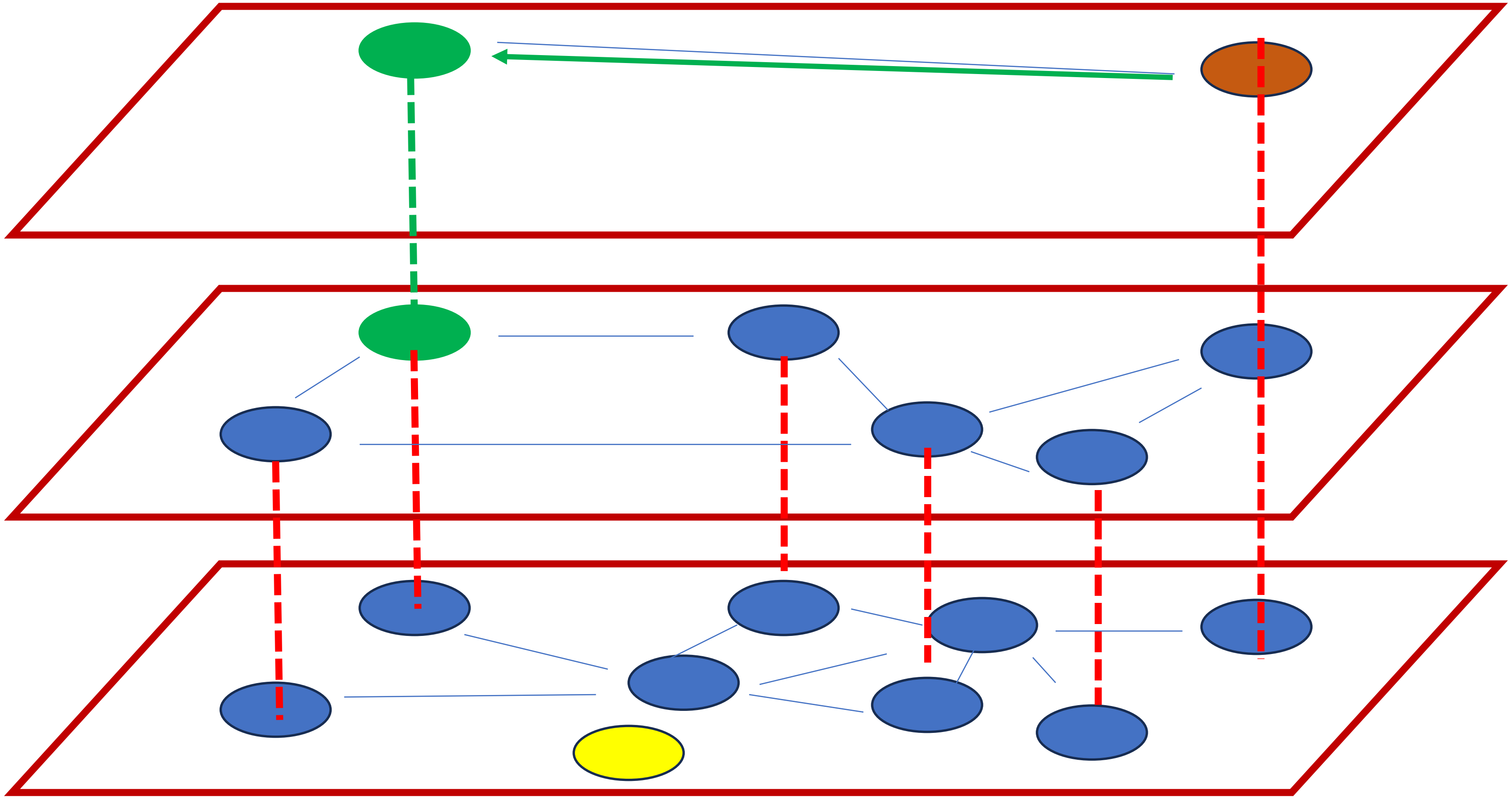
We move to the nearest vertex until we find a local minimum. Unlike NSW, **at this point, we shift to the current vertex in a lower layer and begin searching again**. We repeat this process until finding the local minimum of our bottom layer — layer 0.

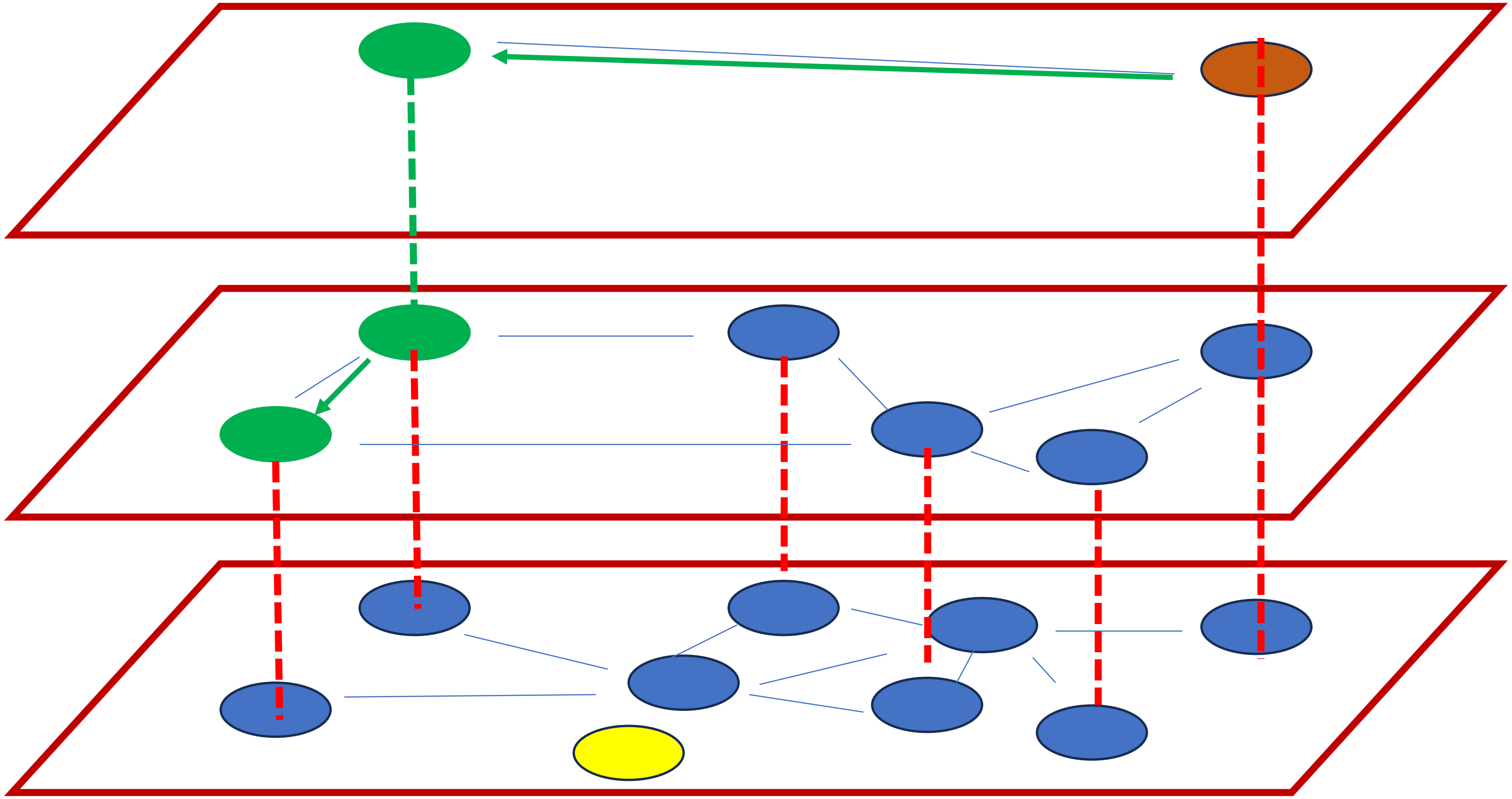


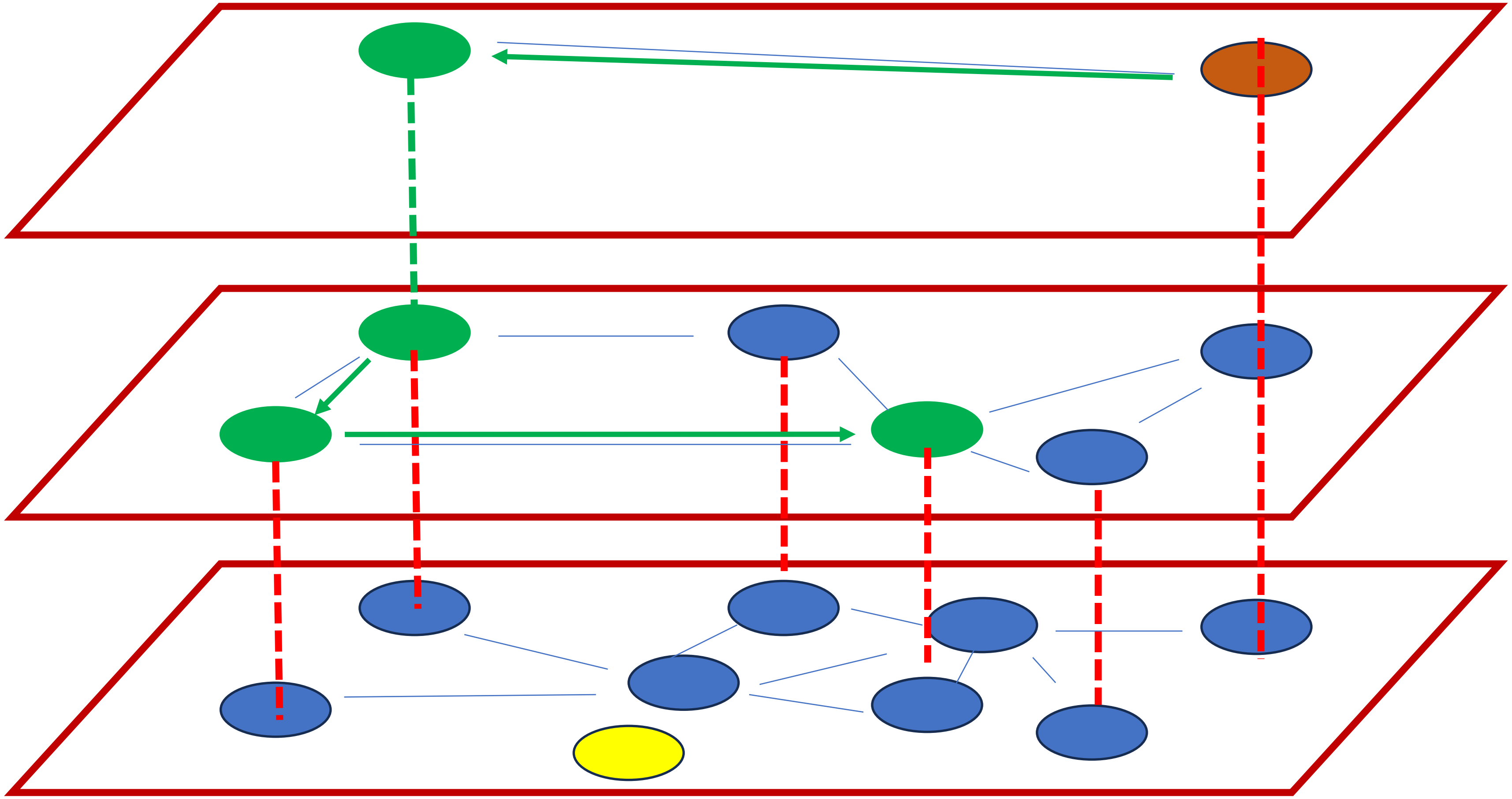
https://www.pinecone.io/learn/series/faiss/hnsw/

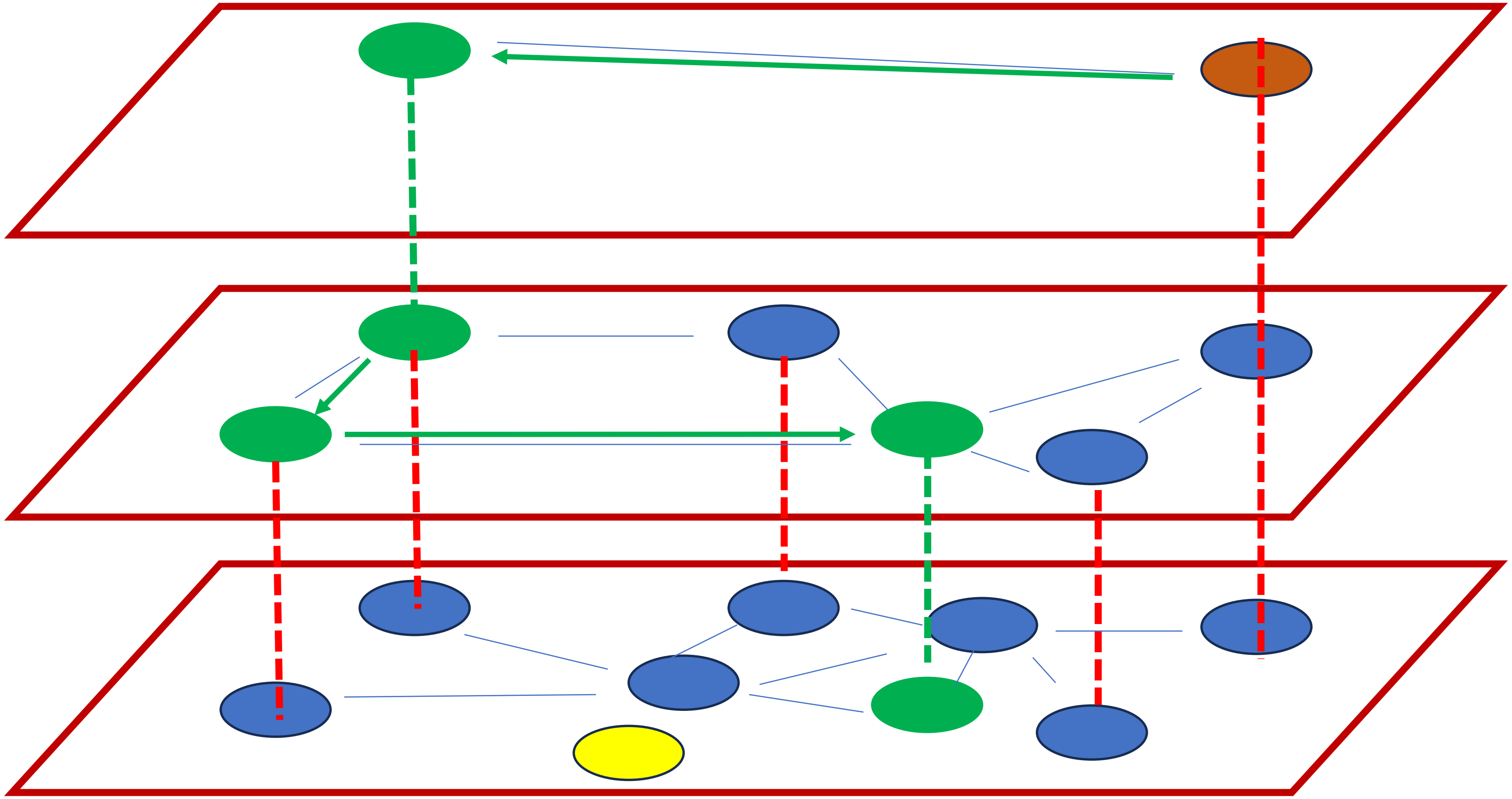

Query

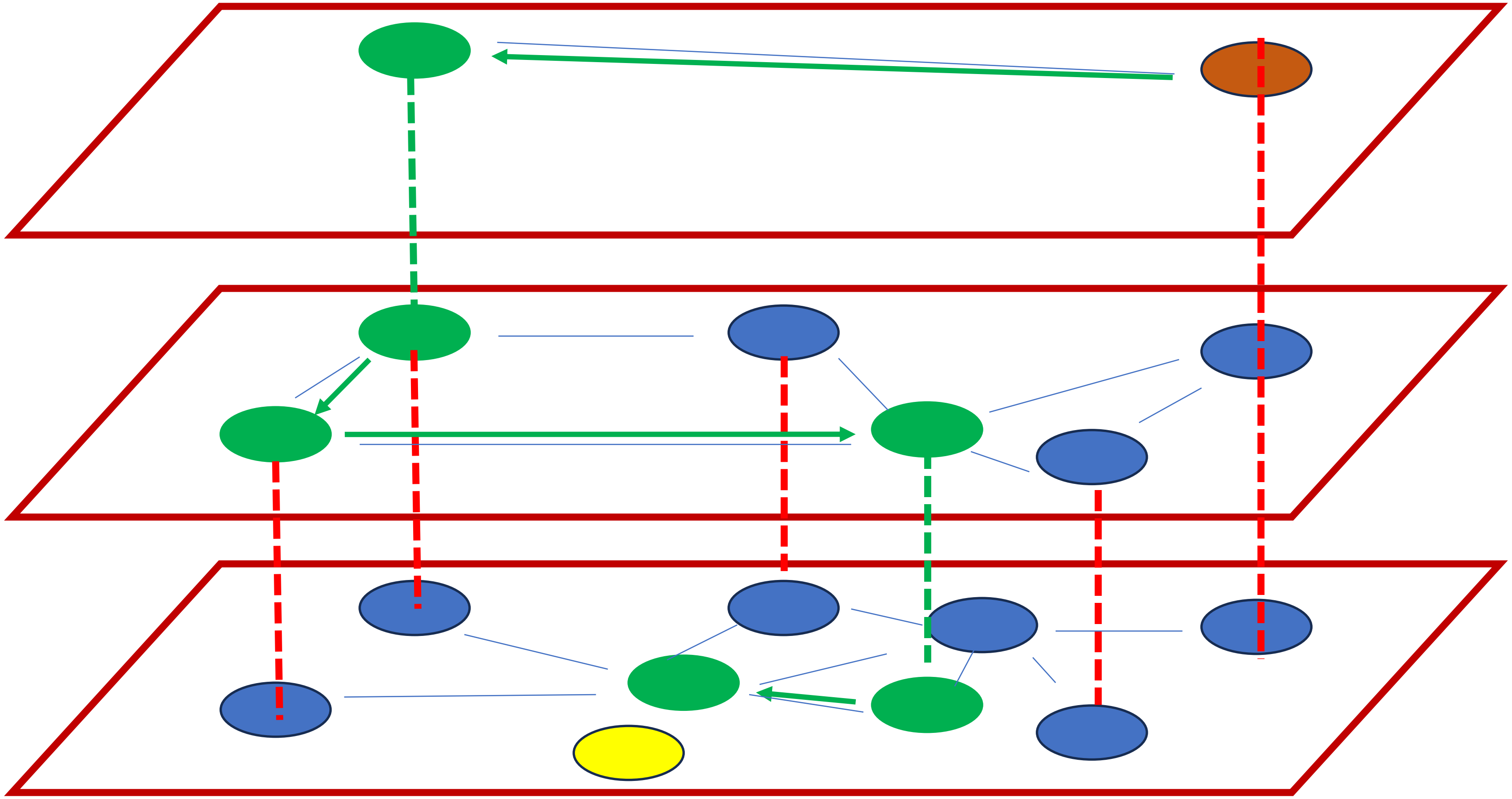








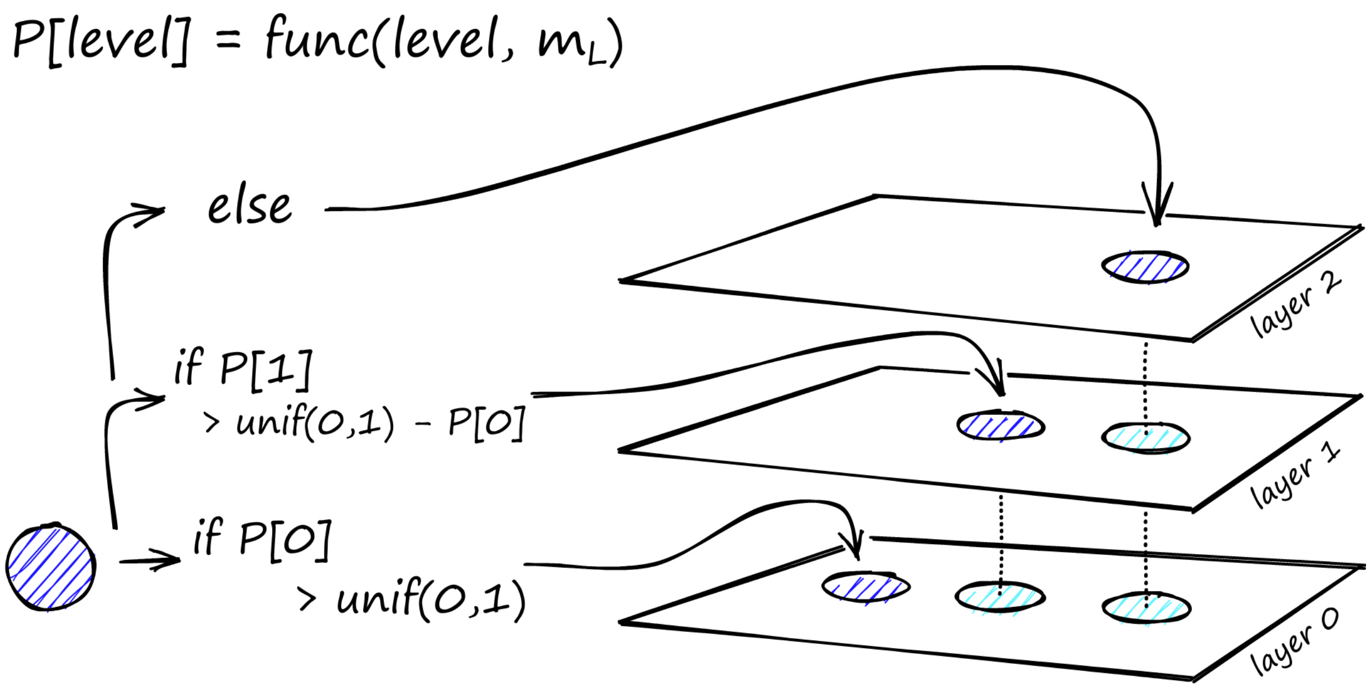




How to construct HNSW graph?

During graph construction, vectors are iteratively inserted one-by-one. The number of layers is represented by **parameter *L***.

The probability of a vector insertion at a given layer is given by a **exponentially decaying probability** function normalized by the ***'level multiplier'*** m_L



The probability function is repeated for each layer (other than layer 0).

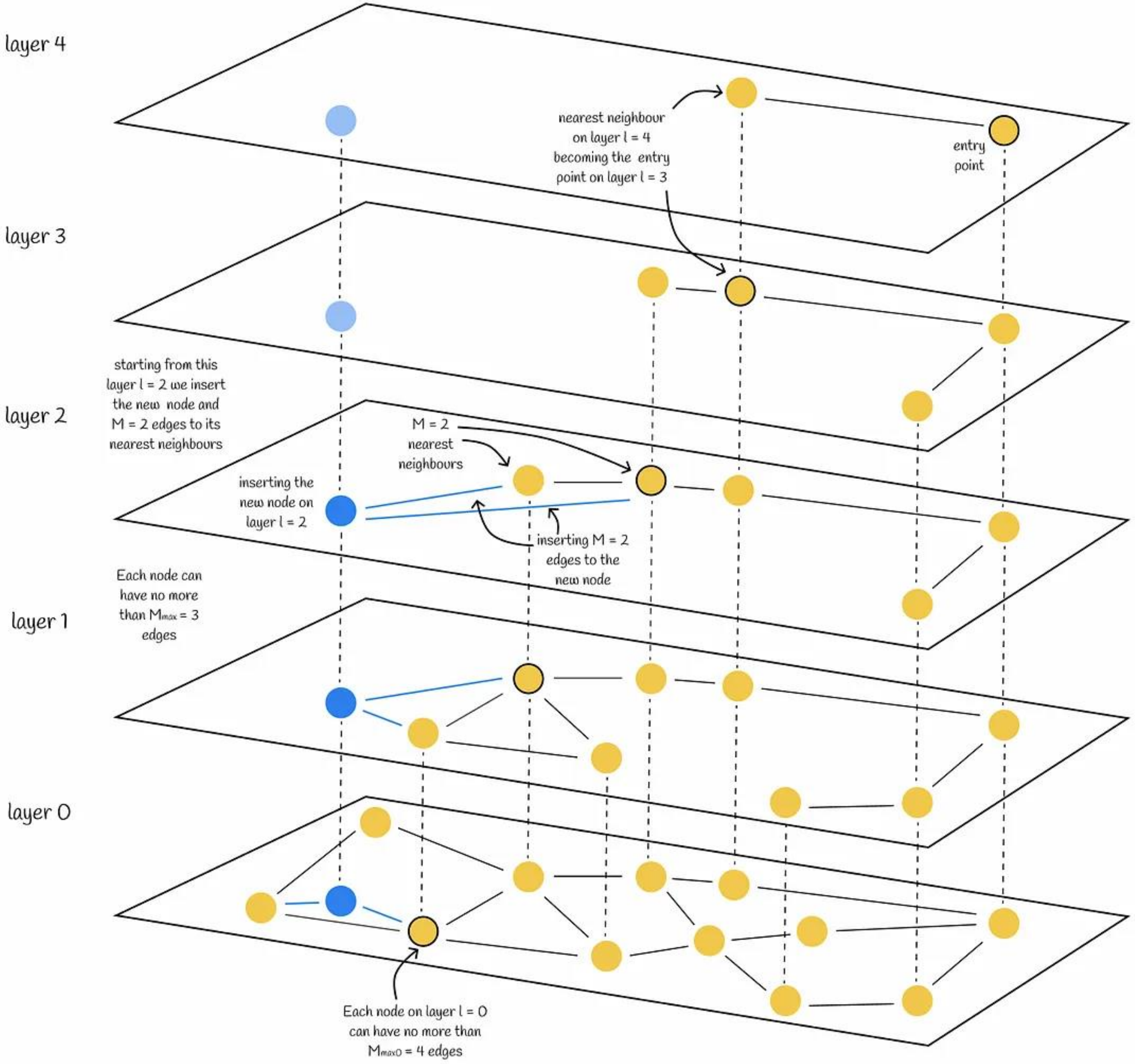
The vector is added to its insertion layer and every layer below it.

Constructing HNSW

After a node is assigned the level number (**value l**), 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.

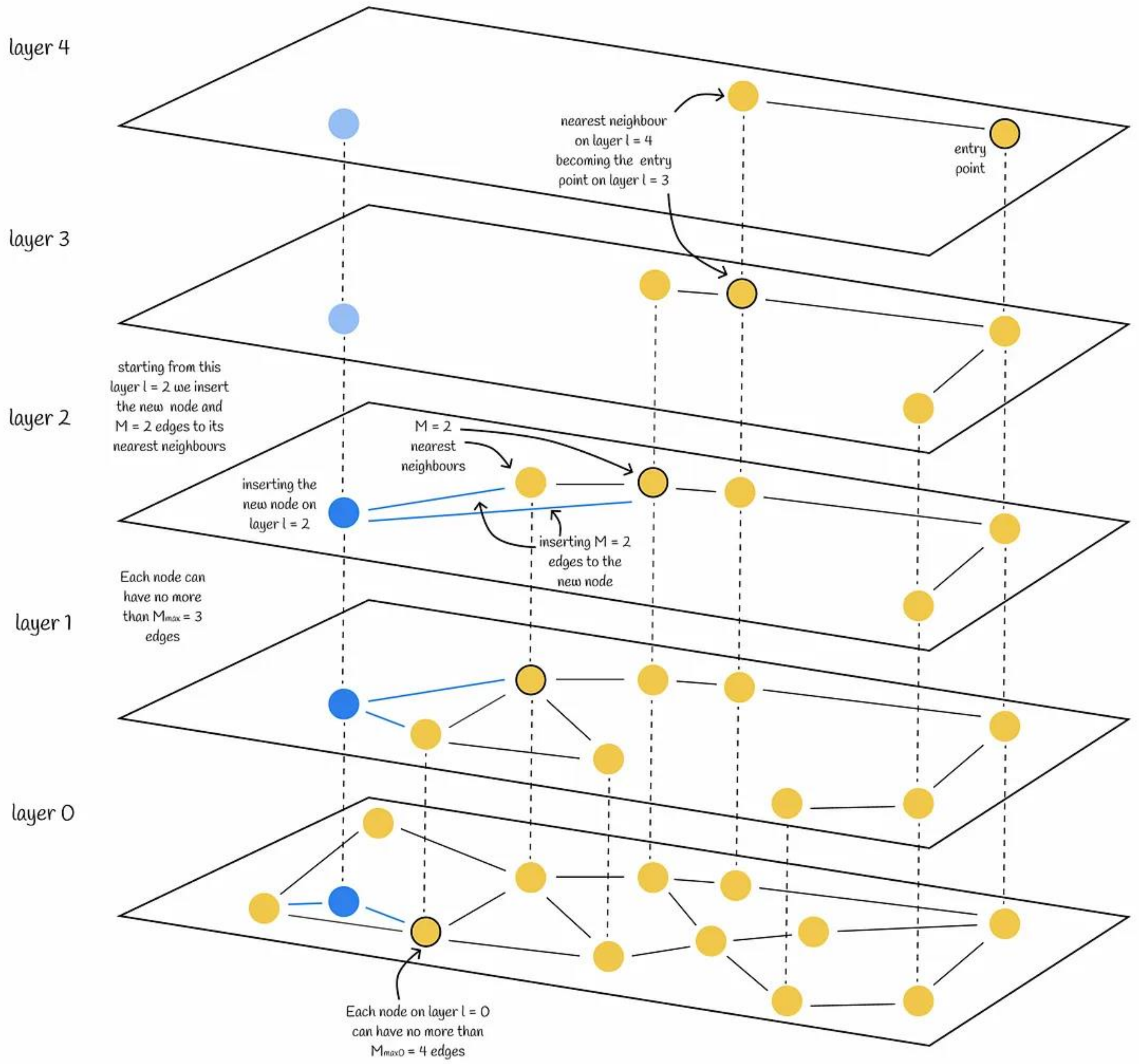


https://towardsdatascience.com/similarity-search-part-4-hierarchical-navigable-small-world-hnsw-2aad4fe87d37

Constructing HNSW

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.

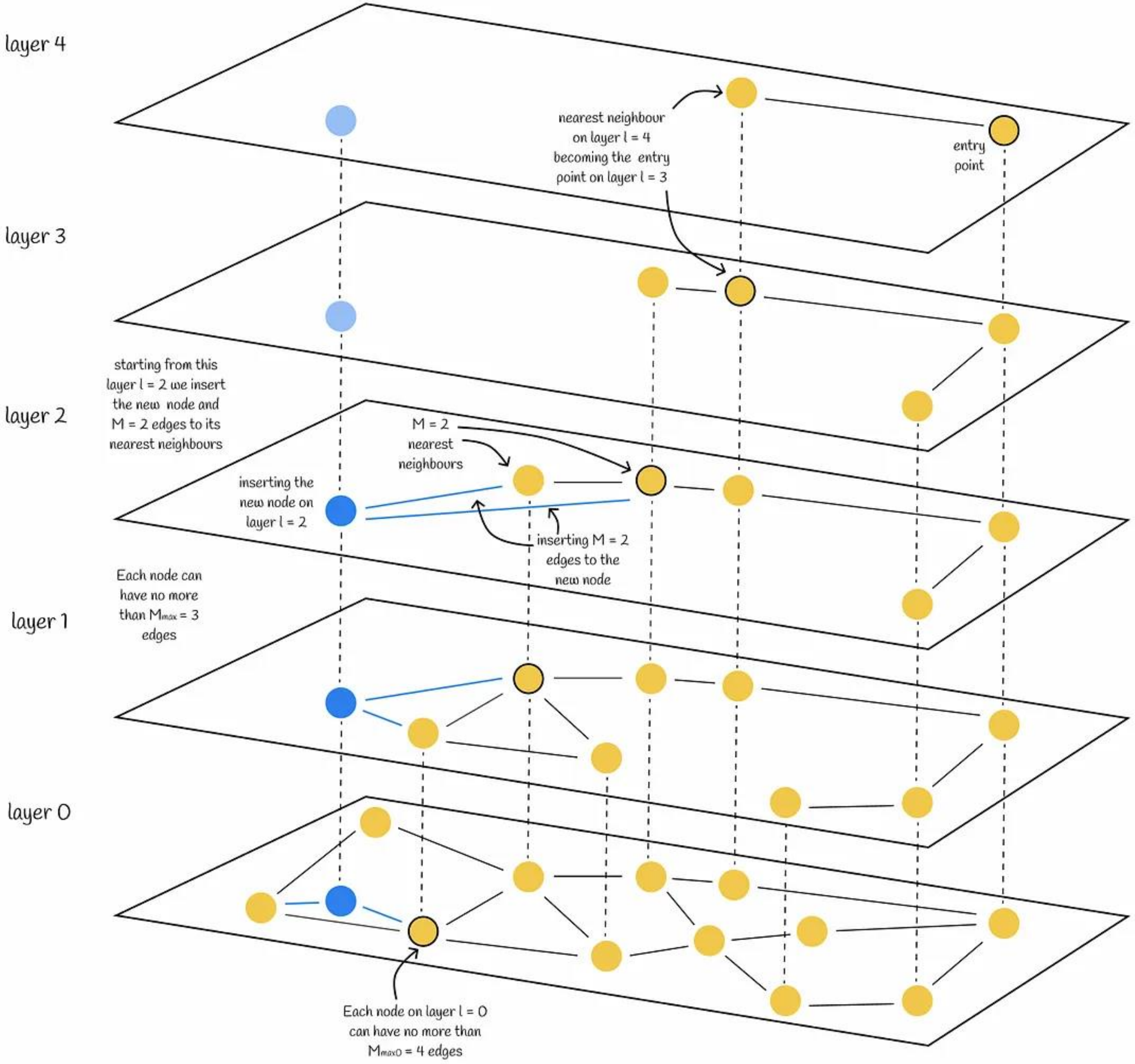


https://towardsdatascience.com/similarity-search-part-4-hierarchical-navigable-small-world-hnsw-2aad4fe87d37

Constructing HNSW

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.



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