

Systems and Methods for Big and Unstructured Data Project

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1 Introduction

Medicines play a pivotal role in healthcare, serving as a cornerstone in the treatment, management, and prevention of diseases, illnesses, and various health conditions. Nowadays, medicines are mass-produced, and all of their meaningful information needs to be organized in some datasets. Such datasets, like the one used in this work, are massive, heterogeneous, and complex and therefore require big data solutions. In particular, a document database like MongoDB is suitable for this type of dataset since documents well represent objects with attributes, just like medicines with their description, cost, manufacturer information, and side effects. Some of these attributes are complex and are either expressed as other objects or arrays of attributes, both well handled by MongoDB via subdocuments and array type. MongoDB does not focus excessively on the relationships among objects, as graph databases do, but they are indeed poor in the present work's data set, nor on text search, as information search-based databases do, but it is not necessary with the existing attributes. Moreover, MongoDB uses a flexible document-based data model that allows for the storage of data in a schema-less manner and is designed for horizontal scalability by supporting sharding, namely allowing the distribution of data across multiple servers or clusters enabling high performance and scalability as data volumes grow: this is important in data sets like the one used in this work where there are hundreds of thousands of instances. It uses also indexing, query optimization, and native, efficient handling of JSON-like documents to enhance performance which is higher than a standard relational database, especially when dealing with huge datasets.



2 Data Wrangling

After obtaining the dataset from its source, several data-wrangling steps were essential to cleanse and transform the data into an analyzable format. This aimed to generate dependable insights and streamline storage within a MongoDB database.

The primary emphasis was on restructuring or cleaning the values within the dataset's columns, outlined below:

1. Removal of currency symbols from the 'product_price' column and converting it into a numeric format. This was accomplished by executing the following code:

2. In the original dataset, the 'side_effects' column contained a string with effects separated by commas. To enhance query flexibility and streamline data organization, this string was split based on commas, resulting in the creation of a new column named 'side_effects_type.' This transformation aimed to convert the data into an array field, enabling more targeted queries for specific side effects. Additionally, this process facilitated essential grouping operations by structuring the side effects in a more accessible format

```
def replace_with_list(row):
    return row['side_effects_type']['side_effect']

# Apply the function to the DataFrame column

df['side_effects_type'] = df.apply(replace_with_list, axis=1)

# Converting the lists to EJSON format

df['side_effects_type'] = df['side_effects_type'].apply(lambda x:
    json.dumps(x))
```

3. The 'salt_composition' column initially combined both the chemical composition and corresponding doses within a single string. To enable separate queries for specific compositions or doses, the field structure was altered. It was transformed into a subdocument field featuring two distinct attributes: 'composition' and 'dose.' This transformation process involved employing regex-based operations to extract the pertinent information.

```
# Extracting text within parentheses and creating a new column
df['salt_composition_dose'] =
     df['salt_composition'].str.extract(r'\((.*?)\)')
 # Removing the extracted content from the 'salt_composition' column
 df['salt_composition'] =
     df['salt_composition'].str.replace(r'\(.*?\)', '').str.strip()
 # Function to process each row in the column
 def transform_row(row):
     # Split the row based on '+'
     elements = [elem.strip() for elem in row.split('+')]
10
     return {"composition": elements}
11
12
# Apply the transformation to each row in the column
 df['salt_composition'] = df['salt_composition'].apply(transform_row)
15
17 def modify_salt_composition(row):
```

- 4. The transformation within the 'drug_interactions' column involved converting the initial single textual field into an array of subdocuments. Each subdocument comprised the following attributes:
 - 'drug': Represents the drug involved in the interaction.
 - 'brand': Corresponds to the brand of the interacting drug. An array containing effect lists. This process aimed to restructure the
 - 'effect': Specifies the level of severity of the interaction.

```
def process_interaction(interaction_string):
     interaction_data = json.loads(interaction_string)
     interactions = []
     min_length = min(len(interaction_data['drug']),
         len(interaction_data['brand']),
         len(interaction_data['effect']))
     for i in range(min_length):
         interaction = {
             'drug': interaction_data['drug'][i],
             'brand': interaction_data['brand'][i],
10
             'effect': interaction_data['effect'][i]
11
         }
12
         interactions.append(interaction)
13
```

```
if len(interaction_data['drug']) !=
         len(interaction_data['brand']) or
         len(interaction_data['drug']) !=
         len(interaction_data['effect']):
         diff1 = len(interaction_data['drug']) - min_length
16
         diff2 = len(interaction_data['brand']) - min_length
17
         diff3 = len(interaction_data['effect']) - min_length
18
19
         for i in range(abs(diff1)):
20
             interactions.append({
21
                 'drug': interaction_data['drug'][min_length + i] if
                    diff1 > 0 else 'nan',
                 'brand': interaction_data['brand'][min_length + i] if
23
                    diff2 > 0 else 'nan',
                 'effect': interaction_data['effect'][min_length + i]
24
                    if diff3 > 0 else 'nan'
             })
25
26
     return {"interactions": interactions}
```

5. The final refinement centered on the 'brand' field within the drug interaction column. Acknowledging the potential existence of multiple associated brands for a specific drug, the decision was made to replace the initial 'brand' attribute, which was a single text field, with an array encompassing all the values. By leveraging a commabased split operation, this transformation resulted in an array containing diverse brand names linked with the drug, offering a more comprehensive and detailed representation of the data.

```
# Function to transform 'brand' column into an array
def transform_brand(brand):
    # If brand contains commas, split by commas and return a list
    if ',' in brand:
        brand_list = [b.strip() for b in brand.split(',')]
        return brand_list
else:
    return [brand] # Return single value as a list
```

2 Data Wrangling 7

```
10 # Function to process 'drug_interactions' column
def process_drug_interactions(interactions):
     # Convert string representation to a dictionary
     interactions_dict = json.loads(interactions)
13
14
     # Transform 'brand' within 'interactions' into an array
     for interaction in interactions_dict['interactions']:
16
         interaction['brand'] = transform_brand(interaction['brand'])
17
18
     # Convert back to Extended JSON (EJSON) format
19
     return json.dumps(interactions_dict)
21
22 # Apply the transformation to the 'drug_interactions' column
23 df['drug_interactions'] =
     df['drug_interactions'].apply(process_drug_interactions)
```



3 Dataset

The dataset used in this work contains information about medications, in particular their descriptions, compositions, drug interactions, side effects, prices, manufacturers, and related details. The dataset contains only medicines used in India, with consequent prices expressed in Indian Rupee and Indian manufacturers.

Its non-relational schema is the following:

```
1 {
   "_id": ObjectId,
    "sub_category": String,
    "product_name": String,
    "salt_composition": Object {
      "composition": Array-[String],
      "dose": String
   },
8
    "product_price": Float,
    "product_manufactured": String,
10
    "medicine_desc": String,
11
    "drug_interactions": Array-[Object] [
12
13
        "drug": String,
        "brand": Array-[String],
15
        "effect": String
16
      }
17
   ],
18
    "side_effects_type": Array-[String]
20 }
```

10 3 Dataset

The structure of the data set is the following: Principle document

- _id (ObjectId): Unique identifier for the medication
- sub_category (String): Sub-category of the medication
- product name (String): Name of the medication
- salt_composition (Object): subdocument containing information about the salt composition of the medication
- product price (Float): Price of the medication
- product manufactured (String): Name of the manufacturer
- medicine_desc (String): Description of the medication
- interactions (Array of Objects): Array of subdocuments containing information about the interactions with the medication
- side_effects_type (Array of Strings): List of side effects associated with the medication

salt composition subdocument

- composition (Array of Strings): List of components in the medication
- dose (String): Dosage information.

interaction subdocument

- drug (String): Name of the drug involved in the interaction
- brand (Array of String): List of brand names of the drug
- effect (String): Description of the effect caused by the drug interaction

For each performed query, a title, a description of what the query is supposed to do, the query itself, and its outcome are provided.

4.0.1. Query 1

Title: Filtered medications by salt composition doses

Description: This query aims to retrieve information about medicines that have a defined price and a specified dose ('30IU' or '60IU'). It then extracts specific fields from matching documents and arranges the results alphabetically by the product names. In particular, the steps are:

- Conditions: using the first parameter of the find() method
 - Price: The query filters for documents where the 'product' price' field exists.
 - Salt composition dose: The query further filters for documents where the 'salt composition.dose' field matches either '30IU' or '60IU'
- Projection: using the second parameter of the find() method, including
 - 'product name
 - 'sub category'
 - 'medicine desc'
 - 'product price'
 - ' id' explicitly excluded
- Sorting: in ascending order based on the 'product' name' field

```
db.getCollection('medicine_data')
   .find(
```

```
{
    product_price: { $exists: true },
        'salt_composition.dose': {
        $in: ['30IU', '60IU']
    }
},
{
    product_name: 1,
    sub_category: 1,
    medicine_desc: 1,
    product_price: 1,
    _id: 0
}
).sort({ product_name: 1 });
```

Query outcome:

```
sub_category: "Actin"
product_name: "Acton Prolongatum 601U Injection"
product_price: 1060.79
medicine_desc: "Acton Prolongatum 601U Injection is an adrenocorticotropic hormone ana."

sub_category: "Antitoxic Sera"
product_name: "Combefive Injection"
product_price: 530.75
medicine_desc: "Combefive Injection is a prescription medicine. This combination of va."

sub_category: "Antitoxic Sera"
product_name: "Convac 3 + BioHib Combipack"
product_price: 330.75
medicine_desc: "Convac 3 + BioHib Combipack"
product_price: 330.36
medicine_desc: "Convac 5 Injection"
product_price: 330.37
medicine_desc: "Convac 5 Injection"
product_price: 330.34
medicine_desc: "Convac 5 Injection is a prescription medicine. This combination of vac."

sub_category: "Antitoxic Sera"
product_mame: "Convac 5 Injection is a prescription medicine. This combination of vac."

sub_category: "Antitoxic Sera"
product_price: 330.34
medicine_desc: "Convac 5 Injection is a prescription medicine. This combination of vac."

sub_category: "All Other Vaccines"
product_price: 330.34
medicine_desc: "Convac 5 Injection is a prescription medicine having combination of va."

sub_category: "All Other Vaccines"
product_price: 327
medicine_desc: "Convac 5 Vaccines"
product_price: 340.42
medicine_desc: "Quinaxaem Vaccines"
product_price: 373.3
medicine_desc: "Quinaxaem Vaccines"
product_price: 373.3
medicine_desc: "Point Vaccines"
product_name: "Quinaxaem Vaccines is a prescription medicine having combination of med."

sub_category: "All Other Vaccines"
product_name: "Quinaxaem Vaccines is a prescription medicine having combination of med."

sub_category: "All Other Vaccines"
product_name: "Tripacel Vaccines is a combination of three vaccines used to prevent dip."
```

4.0.2. Query 2

Title: Filtered medications by salt composition and manufacturer exclusion

Description: This query aims to retrieve information about medications that contain a specific combination of salts (Isoniazid, Pyrazinamide, and Ethambutol) in their composition while excluding medicines manufactured by 'Lupin Ltd' and 'Macleods Pharmaceuticals Pvt Ltd'. It then fetches specific fields from matching documents, focusing on the product name, medicine description, and manufacturer details. In particular, the steps are:

- Conditions: using the first parameter of the find() method
 - Salt composition: It filters documents where the 'salt_composition.composition' field contains all three values: 'Isoniazid', 'Pyrazinamide', and 'Ethambutol'.

 The \$all operator ensures that each of these components is present in the 'composition' array field.
 - Manufacturer: The query further filters based on the 'product_manufactured' field. It excludes documents where the 'product_manufactured' field does not match specific values using the \$nin (not in) operator. In this case, it excludes medicines manufactured by 'Lupin Ltd' and 'Macleods Pharmaceuticals Pvt Ltd'
- Projection: using the second parameter of the find() method, including

```
product_manufactured: {
    $nin: [
        'Lupin Ltd',
        'Macleods Pharmaceuticals Pvt Ltd'
    ]
    }
},
{
    product_name: 1,
    medicine_desc: 1,
    product_manufactured: 1
}
);
```

Query outcome:

```
"id: ObjectId!"650a657302760580228a2b")
product_name: "Mycurit 4 mg Tablet" product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b")
product_name: "Mycurit 4 mg Tablet" product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b")
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b")
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b")
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b")
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b")
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b;
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b;
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b;
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228a2b;
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228b03b0;
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228b03b0;
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228b03b0;)
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228b03b0;)
product_name: "Mycurit 4 mg Tablet is a combination medicine used in the treatment of_"

-id: ObjectId!"650a657302760580228b03
```

4.0.3. Query 3

Title: Filtered medicines by dose and side effects count

Description: This query aims to retrieve information about medications that have a specific salt composition dose ('500mg/5ml') and precisely four side effects listed in their data. It extracts the product name and medicine description from the matching documents. In particular, the steps are:

- Conditions: using the first parameter of the find() method
 - Logical AND Operator: The \$and operator is utilized to specify that both conditions must be satisfied.
 - Salt Composition Dose: The query filters documents where the 'salt_composition.dose' field matches '500mg/5ml'
 - Side Effects Type: It further filters documents where the 'side_effects_type'
 array field has precisely 4 elements
- Projection: using the second parameter of the find() method, including

```
- 'product_name
```

- 'medicine desc'

Query outcome:

```
_id: ObjectId('650a66070dIrdsSB0256210')
product_name: "Pedicloryl Oral Solution'
medicine_desc: "Pedicloryl Oral Solution is a prescription medicine used to treat inso_"

_id: ObjectId('650a66070d2fd5800256480')
product_name: "Pedicloryl Oral Solution'
medicine_desc: "Pedicloryl O
```

4.0.4. Query 4

Title: Medicines with filtered interactions, price, and subcategory

Description: This query aims to retrieve information about medications that meet specific criteria: having 'Alendronic Acid' and 'Aspirin' listed as interactions, a product price less than 100, and belonging to the 'Antacids Antiflatulents And Carminatives' subcategory. It retrieves selected fields and presents the medicine with the lowest price among matching documents. In particular, the steps are:

- Conditions: using the first parameter of the find() method
 - Logical AND Operator: Uses the \$and operator to combine multiple conditions
 - Drug Interactions: Filters for documents where both 'Alendronic Acid' and 'Aspirin' are listed as interactions in the 'drug_interactions' array field

- Product Price: Filters for documents where the 'product_price' exists and is less than 100.

- Subcategory: Filters for documents in the 'Antacids Antiflatulents And Carminatives' subcategory.
- Projection: using the second parameter of the find() method, including

```
- 'product name
```

- 'drug_interactions'
- 'product_price'
- 'sub category'
- Sorting: in ascending order based on 'product' price'
- Limiting: just one for readability purposes

```
db.getCollection('medicine_data')
  .find(
    {
      $and: [
        {
          'drug_interactions.interactions.drug':
            'Alendronic Acid'
        },
        {
          'drug_interactions.interactions.drug':
            'Aspirin'
        },
        { product_price: { $1t: 100 } },
        { product_price: { $exists: true } },
        {
          sub_category:
            'Antacids Antiflatulents And Carminatives'
        }
      ]
    },
    {
```

```
product_name: 1,
    drug_interactions: 1,
    product_price: 1,
    sub_category: 1
  }
)
.sort({ product_price: 1 })
.limit(1);
```

Query outcome:

```
_id: ObjectId('659a65fe0d2fdd58b9248ed2')
 sub_category: "Antacids Antiflatulents And Carminatives"
product_name: "Nodosis GST Tablet"
 product_price: 33.49

    drug_interactions: Object

  * interactions: Array (4)
    ▼ 0: Object
          drug: "Abacavir"
       v brand: Array (3)
0: "Abamune"
            1: "A-Bec"
           2: "Virol"
         effect: "SERIOUS"
     ▼ 1: Object
          drug: "Aspirin"
       ▼ brand: Array (3)
    0: "M Spirin"
    1: "Aspirin"
            2: "Asalite"
          effect: "SERIOUS"
     ▼ 2: Object
          drug: "Adefovir"

▼ brand: Array (3)

          0: "Adesera"
1: "Adheb"
            2: "Adfovir"
          effect: "SERIOUS"
     ▼ 3: Object
          drug: "Alendronic Acid"
       ▼ brand: Array (1)
0: " Alendrate"
          effect: "SERIOUS"
```

4.0.5. Query_5

Title: Filtered medicines by insulin subcategories and manufacturers and specific product exclusion

Description: This query aims to retrieve information about medications based on specific criteria, including different sub-categories of insulin products manufactured by different companies. It then excludes a specific product from the results and the selected fields are projected in the output. In particular, the steps are:

- Conditions: using the first parameter of the find() method
 - Logical AND Operator: Uses the \$and operator to combine multiple conditions.

- Nested OR Conditions: Two sets of conditions within \$or, each representing a combination of sub-category and manufacturer: 'Human Insulin Basal' manufactured by 'Sun Pharmaceutical Industries Ltd', 'Human Insulin Rapid' manufactured by 'Eli Lilly and Company India Pvt Ltd'.

- Product Exclusion: Uses the \$nor operator to exclude documents where the 'product_name' field matches 'Huminsulin R 100IU Cartridge'
- Projection: using the second parameter of the find() method, including

```
- 'sub category'
       - 'product name
       - 'medicine desc'
       - ' id' explicitly excluded
Query:
db.getCollection('medicine_data').find(
  {
    $and: [
      {
        $or: [
          {
             $and: [
               {
                 sub_category:
                    'Human Insulin Basal'
               },
               {
                 product_manufactured:
                    'Sun Pharmaceutical Industries Ltd'
               }
             ]
          },
           {
             $and: [
               {
                 sub_category:
                    'Human Insulin Rapid'
```

```
},
              {
                product_manufactured:
                   'Eli Lilly and Company India Pvt Ltd'
              }
            ]
          }
        ]
      },
      {
        $nor: [
          {
            product_name:
              'Huminsulin R 100IU Cartridge'
          }
        ]
      }
    ]
  },
  {
    sub_category: 1,
    product_name: 1,
    medicine_desc: 1,
    _id: 0
  }
);
```

Query outcome:

["sub_category": "Human Insulin Besal", "product_name": "Insulin 40IU/al Injectio "medicine_desc": "Insulin 40IU/al Injecti }	er, or is used to teprone bland targer control. In adults and diffuse with type 2 and eyes 2 aliebens will time, it is an intermediate secting type of insulin time believe believe bland targer benefit and referre the chance of developing parties on
"sub_category": "Human Insulin Basel", "product_name": "Insucare N 4025/ml Injec	tion, cities to see to improve bland upper central to adults and children with type 2 and type 2 distants million. It is an intermediate retting type of insolin that below to beer bland upper bends not reduce the channel of mentaling series.
"sub_category": "Human Insulin Hapid", "product_name": "Huminsulin R 4022/ml Inj	nation. Species in a short-setting families used to treat type 2 and type 2 dishetes milities. It is used together with a healthy driet and regular energias to content blood super familia after mails. This helps to present serious complications of the
{ "sub_category": "Human Insulin Hapfd", "product_name": "Huminsulin R 1885U/ml is "medicins_desc": "Huminsulin R 1885U/ml is }	laction for injective", solicities for injective, it is abert-certing featile used to creat type 2 and type 2 disheren whiltes. It is used together with a healthy diet and regular exercise to control bland super break after weak. This height to prevent serious couple
"sub_category": "Human Insulin Rapid", "product name": "Humaniert R 1802U/el Inje	ctions, action is a short-acting founds used to cross type 2 and type 2 citatens welltime. It is used tagether with a healthy diet and repolar exercise to control these super benefits after swells, this helps to present serious complications of dis
"sub_category": "Human Insulin Rapid", "product_name": "Humanect 1002W/ml Inject	tier", tier is abertracting foulde used to tract tye 1 and type 2 dishests will his. It is used togather with a healthy that and regular exercise to control bland super limits after medis. This helps to prevent servino complications of dish

4.0.6. Query 6

Title: Medicines with a specific component and a serious drug interaction

Description: This query aims to retrieve information about medications that have a serious drug interaction and contains 'Bupropion'. It fetches the product name and details about drug interactions from up to two matching documents. In particular, the steps are:

- Conditions: using the first parameter of the find() method
 - Drug Interactions: Filters for documents where there is a drug interaction defined as 'SERIOUS' and there is the component 'Bupropion'. This filters documents where a 'drug_interactions.interactions.effect' is 'SERIOUS' and a 'drug_interactions.interactions.drug' is 'Bupropion'
- Projection: using the second parameter of the find() method, including

```
- 'product_name- 'drug interactions'
```

- ' id' explicitly excluded
- Limiting: just two for readability purposes

Query outcome:

```
product_name: "Parkitidin Tablet"
drug_interactions: Object
  ▼ interactions: Array (2)
    ▼ 0: Object
        drug: "Pramipexole"
       • brand: Array (3)
          0: "Pramipex"
          1: "Pramipar"
          2: "Prami"
        effect: "SERIOUS"
    v 1: Object
        drug: "Bupropion"
       brand: Array (3)
          0: "Bupro"
          1: "Bupep"
          2: "Bunocare"
        effect: "MODERATE"
 product_name: "Amantrel Tablet"
drug_interactions: Object

    interactions: Array (2)

    ▼ 0: Object
        drug: "Pramipexole"
       ▼ brand: Array (3)
          0: "Pramipex"
          1: "Pramipar"
          2: "Prami"
        effect: "SERIOUS"
    v 1: Object
        drug: "Bupropion"
      ▼ brand: Array (3)
          0: "Bupro"
          1: "Bupep"
          2: "Bunocare"
        effect: "MODERATE"
```

4.0.7. Query 7

Title: Filtered medicines by interaction type with a certain substance

Description: This query aims to retrieve information about medications that have interactions involving 'Chlorpromazine' with a defined effect as 'LIFE-THREATENING'. It retrieves the product names and details about drug interactions from up to two matching documents. In particular, the steps are:

- Conditions: using the first parameter of the find() method
 - Element Matching: Uses the \$elemMatch operator to find documents where there is an element (interaction) within the 'drug_interactions.interactions' array that matches both conditions:'drug' equals 'Chlorpromazine' and 'effect' equals 'LIFE-THREATENING'
- Projection: using the second parameter of the find() method, including

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```
- 'drug_interactions'
       - '_id' explicitly excluded
  • Limiting: just two for readability purposes
Query:
db.getCollection('medicine_data')
  .find(
    {
      'drug_interactions.interactions': {
        $elemMatch: {
          drug: 'Chlorpromazine',
          effect: 'LIFE-THREATENING'
        }
      }
    },
      product_name: 1,
      drug_interactions: 1,
      _id: 0
    }
  )
  .limit(2);
```

- 'product name

Query outcome:

```
product name: "Terbinaforce Tablet"
* drug interactions: Object
  * interactions: Array (4)
     * 0: Object
         drug: "Amisulpride"
       * brand: Array (3)
0: "Stozen"
           1: "Sulpigold"
            2: "Amisulide"
         effect: "LIFE-THREATENING"
     * 1: Object
         drug: "Aripiprazole"
        * brand: Array (3)
           8: "Arifril"
1: "Biozol"
2: "Elrip"
         effect: "LIFE-THREATENING"
     * 2: Object
         drug: "Chlorpromazine"
       * brand: Array (3)
0: "Karzine"
           1: "Ostil"
            2: "Prom"
         effect: "LIFE-THREATENING"
     * 3: Object
       drug: "Cilostazol"
• brand: Array (1)
           0: " Pencil"
         effect: "LIFE-THREATENING"
 product name: "Fluka 150 Tablet"
* drug_interactions: Object
  * interactions: Array (4)
     * 0: Object
         drug: "Alfuzosin"
       * brand: Array (3)

0: "Efzu"

1: "Alfuzee"

2: "Alfuflo"
         effect: "LIFE-THREATENING"
     * 1: Object
         drug: "Amisulpride"
       * brand: Array (3)

0: "Stozen"

1: "Sulpigold"
            2: "Amisulide"
         effect: "LIFE-THREATENING"
     * 2: Object
          drug: "Aripiprazole"
       · brand: Array (3)
          0: "Arifril"
           1: "Biozol"
            2: "Elrip"
         effect: "LIFE-THREATENING"
     * 3: Object
drug: "Chlorpromazine
       * brand: Array (1)
0: " Karzine"
         effect: "LIFE-THREATENING"
```

4.0.8. Query_8

Title: Medications interacting with two specific substances

Description: This query aims to find medications that have interactions with 'Benazepril' while specifically having an interaction element related to the brand 'Enatol' and the drug 'Enalapril'. It retrieves the product names and details about the drug interactions for one matching document. In particular, the steps are:

• Conditions: using the first parameter of the find() method

- First drug: 'drug_interactions.interactions.drug' matches 'Benazepril'.
- Second drug: 'drug_interactions.interactions' contains an element that matches both the brand 'Enatol' and the drug 'Enalapril'.
- Projection: using the second parameter of the find() method, including
 - 'product name
 - 'drug interactions'
 - ' id' explicitly excluded
- Limiting: to a single document for readability purposes

```
db.getCollection('medicine_data')
  .find(
    {
      'drug_interactions.interactions.drug':
        'Benazepril',
      'drug_interactions.interactions': {
        $elemMatch: {
          brand: 'Enatol',
          drug: 'Enalapril'
        }
      }
    },
      product_name: 1,
      drug_interactions: 1,
      _id: 0
    }
  )
  .limit(1);
```

Query outcome:

```
product_name: "Human Insulatard 40IU/ml Suspension for Injection"
drug_interactions: Object
 ▼ interactions: Array (4)
    ▼ 0: Object
drug: "Benazepril"
       ▼ brand: Array (1)
0: " Apriace"
          effect: "MODERATE"
       1: Object
         drug: "Captopril"
       ▼ brand: Array (3)
           0: "Capotril"
1: "Aceten"
         2: "Angiopril"
effect: "MODERATE"
      2: Object
drug: "Enalapril"
       ▼ brand: Array (3)
0: "Enatol"
            1: "AB-Pril"
2: "Inopril"
         effect: "MODERATE"
      3: Object
  drug: "Fosinopril"
       → brand: Array (1)
    0: " Fovas"
    effect: "MODERATE"
```

4.0.9. Query 9

Title: Affordable manufacturers of a type of medication

Description: This query identifies and presents 10 manufacturers within the 'Ophthal-mological Anti Infectives Medicines' category whose average product price falls at or below 200. In particular, the steps are:

- Match: Filters documents from the 'medicine_data' collection where the 'sub_category' field matches 'Ophthalmological Anti Infectives Medicines'
- Group: Groups the filtered documents by the 'product_manufactured' field, computing the average product price for each manufacturer using the \$avg aggregation operator on the 'product_price' field
- Match: Filters the grouped results to include only those manufacturers whose average product price is less than or equal to 200.
- Limit: Restricts the output to the top 10 results for readability purposes

```
'Ophthalmological Anti Infectives Medicines'
      }
    },
    {
      $group: {
        _id: '$product_manufactured',
        average_product_price: {
          $avg: '$product_price'
        }
      }
    },
    {
      $match: {
        average_product_price: { $1te: 200 }
      }
    },
    { $limit: 10 }
  { maxTimeMS: 60000, allowDiskUse: true }
);
```

Query outcome:

```
PIPELINE OUTPUT
Sample of 10 documents
   _id: "Intas Pharmaceuticals Ltd"
   average_product_price: 142.8
   _id: "Centaur Pharmaceuticals Pvt Ltd"
   average_product_price: 84.57
   _id: "Systopic Laboratories Pvt Ltd"
   average_product_price: 38.6
   _id: "Sun Pharmaceutical Industries Ltd"
   average_product_price: 68.23073359073359
   _id: "Mankind Pharma Ltd"
   average_product_price: 76.8898625
   _id: "Alembic Pharmaceuticals Ltd"
   average_product_price: 59.1688888888888888
   _id: "Torrent Pharmaceuticals Ltd"
   average_product_price: 98.81884857971814
   id: "Abbott"
   average_product_price: 172.84
   _id: "Glaxo SmithKline Pharmaceuticals Ltd"
   average_product_price: 58.23
   _id: "Cipla Ltd"
   average_product_price: 97.1849999999999
```

4.0.10. Query 10

Title: Medications count by a certain manufacturer

Description: This query aims at determining the total count of medications attributed to the manufacturer 'Novo Nordisk India Pvt Ltd'. In particular, the steps are:

- Match: Filters documents from the 'medicine_data' collection where the 'product manufactured' field matches 'Novo Nordisk India Pvt Ltd'
- Group: Counts the number of medications manufactured by this company using the \$sum aggregation operator

```
Query:
```

```
db.getCollection('medicine_data').aggregate(
  {
      $match: {
        product_manufactured:
          'Novo Nordisk India Pvt Ltd'
      }
    },
    {
      $group: {
        _id: 'Novo Nordisk India Pvt Ltd',
        num_of_medications: { $sum: 1 }
      }
    }
 ],
  { maxTimeMS: 60000, allowDiskUse: true }
);
```

Query outcome:

```
_id: "Novo Nordisk India Pvt Ltd" num_of_medications: 62
```

4.0.11. Query 11

Title: Top 10 manufacturers producing the most expensive medications

Description: This query aims to provide insights into manufacturers who produce medications with the highest prices. It groups medications by their respective manufacturers, calculates the maximum price for each, and then sorts these manufacturers based on the highest prices, presenting the top 10 manufacturers producing the most expensive medications. In particular, the steps are:

- Group: Groups the documents from the 'medicine_data' collection by the 'product_manufactured' field and determines the maximum product price for each manufacturer using the \$max aggregation operator on the 'product_price' field. This determines the most expensive product for each manufacturer
- Sort: Sorts the grouped results in descending order based on the 'most_expensive_product' field, arranging manufacturers based on the highest price of their products

Query outcome:

```
_id: "MSD Pharmaceuticals Pvt Ltd"
most_expensive_product: 236500
_id: "BMS India Pvt Ltd"
most_expensive_product: 192238.1
_id: "Roche Products India Pvt Ltd"
most_expensive_product: 111000
_id: "Emcure Pharmaceuticals Ltd"
most_expensive_product: 94999
_id: "Hetero Drugs Ltd"
most_expensive_product: 74200
_id: "Zydus Cadila"
most_expensive_product: 53633.92
_id: "Intas Pharmaceuticals Ltd"
most_expensive_product: 32675.58
_id: "Dr Reddy's Laboratories Ltd"
most_expensive_product: 32675.41
_id: "Psycormedies"
most_expensive_product: 32373.8
_id: "Novartis India Ltd"
most_expensive_product: 25571.4
```

4.0.12. Query 12

Title: Less frequent drug interaction brands in a specific sub-category medicine

Description: This query aims to identify drug interaction brands within the 'Eye Ear Anti Infectives' sub-category that have fewer than 150 occurrences across medicines. It begins by filtering documents related to the specified sub-category, then unwinds arrays associated with drug interactions and brands, counts medicines per brand, and finally filters to identify less frequent drug interaction brands. In particular, the steps are:

- Match: Filters documents where the 'sub_category' field matches 'Eye Ear Anti Infectives'
- Unwind: Deconstructs the 'drug_interactions.interactions' array and 'drug_interactions.interactions.brand' array, creating new documents for each element within these arrays.
- Group: Groups the documents by each unique 'drug_interactions.interactions.brand' and counts the number of medicines associated with each brand using the \$sum aggregation operator
- Match: Filters the grouped results to include only brands with a count of medicines less than 150
- Limit: Limits up to 10 documents for readability purposes

```
path: '$drug_interactions.interactions.brand'
      }
    },
    {
      $group: {
        _id: '$drug_interactions.interactions.brand',
        num_of_medicines_per_brand: { $sum: 1 }
      }
    },
    {
      $match: {
        num_of_medicines_per_brand: { $1t: 150 }
      }
    },
    { $limit: 10 }
 ],
  { maxTimeMS: 60000, allowDiskUse: true }
);
```

```
_id: "Selgelin"
num_of_medicines_per_brand: 84
_id: "Alfuzee"
num_of_medicines_per_brand: 140
_id: "Alestol"
num_of_medicines_per_brand: 140
_id: "Budemon"
num_of_medicines_per_brand: 140
_id: "Astem"
num_of_medicines_per_brand: 140
_id: "Tizakind"
num_of_medicines_per_brand: 84
_id: "Rasalect"
num_of_medicines_per_brand: 84
_id: "Budojet"
num_of_medicines_per_brand: 140
_id: " Doxapress"
num_of_medicines_per_brand: 140
num_of_medicines_per_brand: 140
```

4.0.13. Query 13

Title: Top 10 manufacturers per category with the highest product counts

Description: This query aims to identify and present the top 10 combinations of product categories and manufacturers that have the highest counts of associated products. It groups documents by both the sub-category and manufacturer, calculates the number of products for each combination, and then sorts these combinations based on the highest product counts. In particular, the steps are:

- Group: Groups the documents by a composite identifier consisting of 'sub_category' and 'product_manufactured'. It counts the number of products per combination using the \$sum aggregation operator
- Sort: Sorts the grouped results in descending order based on the count of products ('num_of_products'), ensuring combinations with the highest product counts appear at the top.
- Limit: Limits the output to the top 10 combinations of 'sub_category' and 'product manufactured' with the highest product counts.

```
db.getCollection('medicine_data').aggregate(
  {
      $group: {
        _id: {
          sub_categrory: '$sub_category',
          product_manufactured:
            '$product_manufactured'
        },
        num_of_products: { $sum: 1 }
      }
    },
    { $sort: { num_of_products: -1 } },
    { $limit: 10 }
  ],
  { maxTimeMS: 60000, allowDiskUse: true }
);
```

```
▶ _id: Object
 num_of_products: 4316
▶ _id: Object
 num_of_products: 4308
▶ _id: Object
 num_of_products: 2468
▶ _id: Object
 num_of_products: 2310
▶ _id: Object
 num_of_products: 1904
▶ _id: Object
 num_of_products: 1854
▶ _id: Object
 num_of_products: 1851
▶ _id: Object
 num_of_products: 1851
▶ _id: Object
 num_of_products: 1848
▶ _id: Object
 num_of_products: 1632
```

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4.0.14. Query 14

Title: Manufacturers of Vitamin K Antagonists with low average price

Description: This query aims to identify manufacturers producing 'Vitamin K Antagonists' whose average price across their products falls below 10. It groups documents by both the 'Vitamin K Antagonists' category and manufacturer, calculates the total price for each manufacturer, and filters for those with an average price below the specified threshold. In particular, the steps are:

- Group: Groups the documents by a composite identifier consisting of 'sub_category' (renamed as 'category') and 'product_manufactured'. It calculates the total price for each manufacturer using the \$sum aggregation operator on the 'product_price' field
- Match: Filters the results to include only documents where the '_id.category' is 'Vitamin K Antagonists'
- Match: Further filters the results to consider only those with an 'avg_price' (total price) less than 10
- Project: Projects only the 'product_manufactured' field in the output, renaming the identifier ' id.product_manufactured' as it represents the manufacturer

Query outcome:

```
v _id: Object
    product_manufactured: "Mantri Pharma"

v _id: Object
    product_manufactured: "Harson Laboratories"

v _id: Object
    product_manufactured: "SPM Drugs Pvt Ltd"

v _id: Object
    product_manufactured: "Tabq Therapeutics"
```

4.0.15. Query_15

Title: Drug Interactions with specific components and effect

Description: This query aims to identify and retrieve drug interaction information involving 'Benazepril' with a 'SERIOUS' effect or 'Enalapril' with a 'MODERATE' effect It begins by unwinding the drug interactions, filters for interactions meeting the specified drug and effect conditions, and finally projects the relevant drug interaction details. In particular, the steps are:

- Unwind: Deconstructs the 'drug_interactions.interactions' array, creating a new document for each element within the array
- Match: Filters documents to include only those where the drug interactions meet specific conditions: either 'Benazepril' with a 'SERIOUS' effect or 'Enalapril' with a 'MODERATE' effect
- Project: Projects only the 'drug_interactions' field in the output, retaining information related to the drug interactions

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• Limit: 10 for readability purposes

```
Query:
```

```
db.getCollection('medicine_data').aggregate(
  {
      $unwind: {
        path: '$drug_interactions.interactions'
      }
    },
    {
      $match: {
        $or: [
          {
            \verb|'drug_interactions.interactions.drug'|:
              'Benazepril',
            'drug_interactions.interactions.effect':
              'SERIOUS'
          },
          {
            'drug_interactions.interactions.drug':
              'Enalapril',
            'drug_interactions.interactions.effect':
              'MODERATE'
          }
        ]
      }
    },
    { $project: { drug_interactions: 1 } },
    { $limit: 10 }
  ],
  { maxTimeMS: 60000, allowDiskUse: true }
);
```

```
_id: ObjectId('659a65f10d2fdd58b9236121')
drug_interactions: Object

    interactions: Object
drug: "Enalapril"

      orug: "Enatapril"

→ brand: Array (3)

Θ: "Enatol"

1: "AB-Pril"

2: "Inopril"

effect: "MODERATE"
   _id: ObjectId('659a65f18d2fdd58b9236122')

    drug_interactions: Object

   • interactions: Object
      drug: "Enalapril"
• brand: Array (3)
• "Enatol"
1: "AB-Pril"
2: "Inopril"
          effect: "MODERATE"
   _id: ObjectId('659a65f18d2fdd58b9236123')

    drug_interactions: Object

   * interactions: Object
      Interactions: Object
drug: "Enalapril"
* brand: Array (3)
0: "Enatol"
1: "AB-Pril"
2: "Inopril"
effect: "MODERATE"
_id: ObjectId('659a65f10d2fdd58b9236124')
* drug_interactions: Object
   • interactions: Object
         drug: "Enalapril"
      * brand: Array (3)

0: "Enatol"

1: "AB-Pril"

2: "Inopril"
          effect: "MODERATE"
   _id: ObjectId('659a65f18d2fdd58b9236125')
▼ drug_interactions: Object

→ interactions: Object

      drug: "Enalapril"

• brand: Array (3)

0: "Enatol"

1: "AB-Pril"

2: "Inopril"

effect: "MODERATE"
```

4.0.16. Query 16

Title: Average price per drug interaction brand

Description: This query aims to compute and present the average price per drug interaction brand. It starts by filtering documents with existing product prices, then unwinds arrays related to drug interactions and their associated brands, calculates the average price for each brand, and finally limits the output to the top 10 brands based on their average prices. In particular, the steps are:

- Match: Filters documents where 'product price' field exists
- Unwind: Deconstructs the 'drug_interactions.interactions' array and 'drug_interactions.interactions.brand' array, creating new documents for each element within these arrays
- Group: Groups the documents by each unique 'drug_interactions.interactions.brand' and calculates the average product price for each brand using the \$avg aggregation operator
- Limit: Limits the output to the top 10 drug interaction brands based on their average price

```
db.getCollection('medicine_data').aggregate(
  {
      $match: { product_price: { $exists: true } }
    },
    {
      $unwind: {
        path: '$drug_interactions.interactions'
      }
    },
    {
      $unwind: {
        path: '$drug_interactions.interactions.brand'
      }
    },
    {
```

```
$group: {
    _id: '$drug_interactions.interactions.brand',
    avg_price_per_brand: {
        $avg: '$product_price'
     }
    }
},
{ $limit: 10 }
],
{ maxTimeMS: 60000, allowDiskUse: true }
);
```

```
_id: "Virosine DR"
avg_price_per_brand: 251.9156
_id: "Vagimoist"
avg_price_per_brand: 10.35
_id: " Carz"
avg_price_per_brand: 10.35
_id: "Carz"
_id: "Estratag"
avg_price_per_brand: 10.35
_id: "Sibolone"
avg_price_per_brand: 10.35
_id: "Macbutin"
avg_price_per_brand: 210.3025
_id: "Avifam"
avg_price_per_brand: 1643.4
_id: "Triptam"
avg_price_per_brand: 256.525
_id: "Becoride"
avg_price_per_brand: 285.3188060116894
```

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4.0.17. Query_17

Title: Top 10 side effects and their occurrences

Description: This query aims to retrieve information about medications that have a specific salt composition dose ('500mg/5ml') and precisely four side effects listed in their data. It extracts the product name and medicine description from the matching documents. In particular, the steps are:

- Unwind: Deconstructs the 'side_effects_type' array, creating a new document for each element within the array
- Group: Groups the documents by each unique 'side_effects_type', counting the occurrences of each side effect using the \$sum aggregation operator
- Sort: Sorts the grouped results in descending order based on the count of occurrences ('tot'), ensuring the side effects with the highest frequencies appear at the top
- Limit: Limits the output to the top 10 side effects with the highest occurrences

Query outcome:

```
id: "Nausea"
tot: 17299
id: "Diarrhea"
tot: 14462
_id: "Vomiting"
tot: 11702
_id: "Hypoglycemia (low blood glucose level)"
id: "Headache"
tot: 5103
_id: "Stomach pain"
tot: 4973
_id: "Taste change"
tot: 3613
_id: "Rash"
tot: 3372
_id: "Allergic reaction"
_id: "Upper respiratory tract infection"
```

4.0.18. Query_18

Title: Minimum average price among salt compositions

Description: This query aims to find and present the minimum average price among different salt compositions. It starts by unwinding the compositions, calculates the average price for each composition, and then determines the minimum average price across all these compositions. In particular, the steps are:

- Conditions: using the first parameter of the find() method
 - Logical AND Operator: The \$and operator is utilized to specify that both conditions must be satisfied.
 - Salt Composition Dose: The query filters documents where the 'salt_composition.dose' field matches '500mg/5ml'

- Side Effects Type: It further filters documents where the 'side_effects_type' array field has precisely 4 elements
- Projection: using the second parameter of the find() method, including
 - 'product name
 - 'medicine desc'

Query:

```
db.getCollection('medicine_data').aggregate(
  {
      $unwind: {
        path: '$salt_composition.composition'
      }
    },
    {
      $group: {
        _id: '$salt_composition.composition',
        avg_price_per_composition: {
          $avg: '$product_price'
        }
      }
    },
    {
      $group: {
        _id: 'minimum',
        min_avg_price_per_composition: {
          $min: '$avg_price_per_composition'
        }
      }
    }
  ],
  { maxTimeMS: 60000, allowDiskUse: true }
);
```

_id: "minimum"
min_avg_price_per_composition: 2.12

4.0.19. Query_19

Title: Top 10 product-composition-side effect combinations

Description: This query aims to identify and present the top 10 combinations of product compositions and side effects with the highest occurrences. It unwinds both the composition and side effects arrays, groups documents based on these combinations, calculates the total number of products associated with each combination, and finally limits the output to the top 10 combinations. In particular, the steps are:

- Unwind: Deconstructs the 'salt_composition.composition' array and 'side_effects_type' array, creating new documents for each element within these arrays
- Group: Groups the documents based on combinations of 'salt_composition.composition' and 'side_effects_type'. It calculates the total number of products associated with each composition-side effect combination using the \$sum aggregation operator
- Limits the output to the top 10 combinations of product compositions and side effects with the highest occurrence counts

}

```
},
     { $limit: 10 }
  ],
  { maxTimeMS: 60000, allowDiskUse: true }
);
Query outcome:
                        ▶ _id: Object
                          totproduct_with_side_effect: 4830
                        ▶ _id: Object
                          \verb|totproduct_with_side_effect: 210|\\
                        ▶ _id: Object
                          totproduct_with_side_effect: 4
                        ▶ _id: Object
                          totproduct_with_side_effect: 630
                        ▶ _id: Object
                         totproduct_with_side_effect: 600
                        • _id: Object
                          totproduct_with_side_effect: 210
                        • _id: Object
                          totproduct_with_side_effect: 3
                        ▶ _id: Object
                          totproduct_with_side_effect: 30
                        ▶ _id: Object
                          totproduct_with_side_effect: 420
                        ▶ _id: Object
                          totproduct_with_side_effect: 6
```

4.0.20. Query 20

Title: Top 10 drug compositions with most duplicated side effects

Description: This query aims to identify and present the top 10 drug compositions with the most occurrences of unique duplicated side effects. It performs the unwinding of arrays, groups documents by drug composition and side effects, calculates counts, and then sorts and limits the output to the top 10 compositions. In particular, the steps are:

- Unwind: Deconstructs the 'side_effects_type' array and 'salt_composition' array, creating new documents for each element within these arrays.
- Group: Groups the documents based on combinations of 'salt_composition.composition' and 'side_effects_type'. It calculates the count of duplicated side effects associated with each drug composition
- Groups the results by the drug compositions and calculates the total count of unique duplicated side effects for each drug composition
- Sort: Sorts the grouped results in descending order based on the count of unique duplicated side effects ('right_sum'), ensuring the compositions with the most duplicated side effects are at the top
- Limit: Limits the output to the top 10 drug compositions with the highest counts of unique duplicated side effects

```
'$side_effects_type'
        },
        count_dup: { $sum: 1 }
      }
    },
    {
      $group: {
        _id: '$_id.drug_composition',
        right_sum: { $sum: 1 }
      }
   },
    { $sort: { right_sum: -1 } },
    { $limit: 10 }
 ],
 { maxTimeMS: 60000, allowDiskUse: true }
);
```

```
_id: "Metformin"
right_sum: 20
_id: "Rifampicin"
right_sum: 18
_id: "Pyrazinamide"
right_sum: 17
_id: "Ivermectin"
right_sum: 16
_id: "Isoniazid"
right_sum: 16
_id: "Ethambutol"
right_sum: 16
_id: "Diloxanide"
right_sum: 14
_id: "Dehydroemetine"
right_sum: 12
_id: "Vildagliptin"
right_sum: 12
_id: "Tinidazole"
right_sum: 12
```