Data Design Patterns

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Note: this document is in progress...

The goal of this paper/chapter is to present Data Design Patterns in an informal way.

The emphasis has been on pragmatism and practicality.

Data Design Patterns formats:

- PDF version
- Marcdown version

Source code for Data Design Patterns are provided in GitHub.

Data Design Patterns can be categorized as:

- Summarization Patterns
- In-Mapper-Combiner Pattern
- Filtering Patterns
- Organization Patterns
- Join Patterns
- Meta Patterns
- Input and Output Patterns

1. Summarization Patterns

Typically, Numerical Summarizations are big part of Summarization Patterns. Numerical summarizations are patterns, which involves calculating aggregate statistical values (minimum, maximum, average, median, standard deviation, ...) over data. If data has keys (such as department identifier, gene identifiers, or patient identifiers), then the goal is to group records by a key field and then you calculate aggregates per group such as minimum, maximum, average, median, or standard deviation. If data does not have keys, then you compute the summarization over entire data without grouping.

The main purpose of summarization patters is to summarize lots of data into meaningful data structures such as tuples, lists, and dictionaries.

Some of the Numerical Summarizations patterns can be expressed by SQL. For example, Let gene_samples be a table of (gene_id, patient_id, biomarker_value). Further, assume that we have about 100,000 unique gen_id (s), a patient (represented as patient_id) may have lots of gene records with an associated biomarker value (s).

This Numerical Summarizations pattern corresponds to using GROUP BY in SQL for example:

```
SELECT MIN(biomarker_value), MAX(biomarker_value), COUNT(*)
FROM gene_samples
GROUP BY gene_id;
```

Therefore, in this example, we find a triplet (min, max, count) per gene_id.

In Spark, this summarization pattern can be implemented by using RDDs and DataFrames. In Spark, (key, value) pair RDDs are commonly used to group by a key (in our example gene id) in order to calculate aggregates per group.

Let's assume that the input files are CSV file(s) and further assume that input records have the following format:

```
<gene_id><,><patient_id><,><biomarker_value>
```

RDD Example using groupByKey()

We load data from CSV file(s) and then create an RDD[(key, value)], where key is

gene_id and value is a biomarker_value. To solve it by the reduceByKey(), we first need to map it to a desired data type of (min, max, count):

```
# rdd : RDD[(gene_id, biomarker_value)]
mapped = rdd.mapValues(lambda v: (v, v, 1))
```

Then we can apply <code>groupByKey()</code> transformation:

```
# grouped : RDD[(gene_id, Iterable<biomarker_value>)]
grouped = mapped.groupByKey()
# calculate min, mx, count for values
triplets = grouped.mapValues(
   lambda values: (min(values), max(values), len(values)
)
```

The <code>groupByKey()</code> might give OOM errors if you have too many values per key (<code>gene_id</code>) and <code>groupByKey()</code> does not use any combiners at all. Overall <code>reduceByKey()</code> is a better scale-out solution than <code>groupByKey()</code>.

RDD Example using reduceByKey()

We load data from CSV file(s) and then create an RDD[(key, value)], where key is gene_id and value is a biomarker_value. To solve it by the reduceByKey(), we first need to map it to a desired data type of (min, max, count):

```
# rdd : RDD[(gene_id, biomarker_value)]
mapped = rdd.mapValues(lambda v: (v, v, 1))
```

Then we can apply reduceByKey() transformation:

```
# x = (min1, max1, count1)
# y = (min2, max2, count2)
reduced = mapped.reduceByKey(
    lambda x, y: (min(x[0], y[0]), max(x[1], y[1]), x[2]+y[2])
)
```

Spark's reduceByKey() merges the values for each key using an associative and commutative reduce function.

RDD Example using combineByKey()

We load data from CSV file(s) and then create an RDD[(key, value)], where key is gene id and value is a biomarker value.

RDD.combineByKey(createCombiner, mergeValue, mergeCombiners) is a generic function to combine the elements for each key using a custom set of aggregation functions. Turns an RDD[(K, V)] into a result of type RDD[(K, C)], for a "combined type" C. Note that depending on your data requirements, combined data type can be a simple data type (such as integer, string, ...) or it can be collection (such as set, list, tuple, array, or dictionary) or it can be custom data type.

Users provide three functions:

```
    createCombiner:
    which turns a V into a C (e.g., creates a one-element list)
    mergeValue:
    to merge a V into a C (e.g., adds it to the end of a list)
    mergeCombiners:
    to combine two C's into a single one (e.g., merges the lists)
```

here is the solution by combineByKey():

```
# rdd : RDD[(gene_id, biomarker_value)]
combined = rdd.combineByKey(
    lambda v: (v, v, 1),
    lambda C, v: (min(C[0], v), max(C[1], v), C[2]+1),
    lambda C, D: (min(C[0], D[0]), max(C[1], D[1]), C[2]+D[2])
)
```

DataFrame Example

After reading input, we can create a DataFrame as:

```
DataFrame[(gene_id, patient_id, biomarker_value)]
```

The other alternative solution is to use pure SQL: register your DataFrame as a table, and then fire a SQL query:

Note that your SQL statement will be executed as a series of mappers and reducers behind the Spark engine.

Data Without Keys - using DataFrames

You might have some numerical data without keys and then you might be interested in computing some statistics such as (min, max, count) on the entire data. In these situations, we have more than couple of options: we can use mapPartitions() transformation or use reduce() action (depending on the format and nature of input data).

We can use Spark's built in functions to get aggregate statistics. Here's how to get mean and standard deviation.

```
# import required functions
from pyspark.sql.functions import col
from pyspark.sql.functions import mean as _mean
from pyspark.sql.functions import stddev as _stddev

# apply desired functions
collected_stats = df.select(
    _mean(col('numeric_column_name')).alias('mean'),
    _stddev(col('numeric_column_name')).alias('stddev')
).collect()

# extract the final results:
final_mean = collected_stats[0]['mean']
final_stddev = collected_stats[0]['stddev']
```

Data Without Keys - using RDDs

If you have to filter your numeric data and perform other calculations before omputing mean and std-dev, then you may use RDD.mapPartitions() transformations. The RDD.mapPartitions(f) transformation returns a new RDD by applying a function f() to each partition of this RDD. Finally, you may reduce() the result of RDD.mapPartitions(f) transformation.

To understand RDD.mapPartitions(f) transformation, let's assume that your input is a set of files, where each record has a set of numbers separated by comma (note that each record may have any number of numbers: for example one record may have 5 numbers and another record might have 34 numbers, etc.):

```
<number><,><number><,>...<,><number>
```

Suppose the goal is to find

```
(min, max, count, num_of_negatives, num_of_positives) for the entire data
set. One easy solution is to use

RDD.mapPartitions(f), where f() is a function which returns

(min, max, count, num_of_negatives, num_of_positives) per partition. Once
mapPartitions() is done, then we can apply the final reducer to find the final

(min, max, count, num_of_negatives, num_of_positives) for all partitions.
```

Let rdd denote RDD[String], which represents all input records.

First we define our custom function <code>compute_stats()</code>, which accepts a partition and returns

(min, max, count, num of negatives, num of positives) for a given partition.

```
def count_neg_pos(numbers):
    neg_count, pos_count = 0, 0
    # iterate numbers
    for num in numbers:
        if num > 0: pos_count += 1
        if num < 0: neg_count += 1</pre>
    #end-for
    return (neg count, pos count)
#end-def
def compute_stats(partition):
    first_time = True
    for e in partition:
        numbers = [int(x) for x in e.split(',') if x]
        neg_pos = count_neg_pos(numbers)
        #
        if (first_time):
            min = min(numbers)
            _max = max(numbers)
            _count = len(numbers)
            _neg = neg_pos[0]
            _{pos} = neg_{pos}[1]
            first_time = False
        else:
            # it is not the first time:
            _min = min(_min, min(numbers))
            _max = max(_max, max(numbers))
            _count += len(numbers)
            _neg += neg_pos[0]
            _pos += neg_pos[1]
        #end-if
    #end-for
    return [(_min, _max, _count, _neg, _pos)]
#end-def
```

After defining compute_stats(partition) function, we can now apply the mapPartitions() transformation:

```
mapped = rdd.mapPartitions(compute_stats)
```

```
Now mapped is an RDD[(int, int, int, int, int)]
```

Next, we can apply the final reducer to find the final

```
(min, max, count, num_of_negatives, num_of_positives) for all partitions:
```

Spark is so flexiable and powerful: therefore we might find multiple solutions for a given problem. But what is the optimal solution? This can be handled by testing your solutions against real data which you might use in the production environments. Test, test, and test.

2. In-Mapper-Combiner Design Pattern

In this section, I will discuss In-Mapper-Combiner design patterns and show some examples for using the pattern.

In a typical MapReduce paradigm, mappers emit (key, value) pairs and once all mappers are done, the "sort and shuffle" phase prepare inputs (using output of mappers) for reducers in the form of (key, Iterable<value>), finally, reducers consume these pairs and create final (key, aggregated-vale). For example if mappers have emitted the following (key, vlaue) pairs:

```
(k1, v1), (k1, v2), (k1, v3), (k1, v4), (k2, v5), (k2, v6)
```

Then "sort and shuffle" will prepare the following (key, vlaue) pairs to be consumed by reducers:

```
(k1, [v1, v2, v3, v4])
(k2, [v5, v6])
```

For some data applications, it is very possible to emit too many (key, value) pairs, which may create huge network traffic in the cluster. If a mapper creates the same key multiple times (with different values) for the input partition, then for some aggregation algorithms, it is possible to aggregate/combine these (key, values) and emit less (key, value) pairs. The simplest case is that counting DNA bases (count A's, T's, C's, G's). In a typical MapReduce paradigm, for a DNA string of "AAAATTTCCCGGAAATGG", a mapper will create the following (key, value) pairs:

```
(A, 1), (A, 1), (A, 1), (A, 1), (T, 1), (T, 1), (T, 1), (C, 1), (C, 1), (G, 1), (G 1), (A, 1),
```

For this specific algorithm (DNA base count), it is possible to combine values for the same key:

```
(A, 7), (T, 4), (C, 3), (G, 4)
```

Combining/merging/reducing 18 (key, value) pairs into 4 combined (key, value) pairs is called "In-Mapper-Combining": we combined values in the mapper processing: the advantage is we emit/create much less (key, value) pairs, which will ease the cluster network traffic. The "In-Mapper Combiner" emits (A, 7) instead of 7 pairs of (A, 1) and so on. The In-Mapper-Combiner design pattern is introduced to address some issues (to limit the number of (key, value) pairs generated by mappers) with MapReduce programming paradigm.

When do you need In-Mapper-Combiner design pattern? When your mapper generates too many (key, value) pairs and you have a chance to combine these (key, value) pairs into a smaller number of (key, value) pairs, then you may use In-Mapper-Combiner design pattern.

Informally, say that your mapper has created 3 keys with multiple (key, value) as:

```
key k1: (k1, u1), (k1, u2), (k1, u3), ...
key k2: (k2, v1), (k2, v2), (k2, v3), ...
key k3: (k3, t1), (k3, t2), (k3, t3), ...
```

Then In-Mapper-Combiner design pattern should combine these into the following (key, value) pairs:

```
(k1, combiner_function([u1, u2, u3, ...])
(k2, combiner_function([v1, v2, v3, ...])
(k3, combiner_function([t1, t2, t3, ...])
```

```
Where combiner_function([a1, a2, a3, ...]) is a custom function, which combines/reduces [a1, a2, a3, ...] into a single value.
```

Applying In-Mapper-Combiner design pattern may result in a more efficient algorithm implementation from the performance point (for example reducing time complexity). The <code>combiner_function()</code> must guarantee that it is a semantic-preserving function: meaning that semantic/correctness of algorithms (with and without In-Mapper-Combiner) for mappers must not change at all. The In-Mapper-Combiner design pattern might substantially reduce both the number and size of <code>(key, value)</code> pairs that need to be shuffled from the mappers to the reducers.

Example: DNA Base Count Problem

What is a DNA Base Counting? The four bases in DNA molecule are adenine (A), cytosine (C), guanine (G), and thymine (T). So, a DNA String is comprised of 4 base letters {A, T, C, G}. DNA Base Count finds frequency of base letters for a given set of DNA strings.

Input Format: FASTA

There are multiple text formats to represent DNA. The FASTA is a text based format to represent DNA data. The FASTA file format is a widely used format for specifying biosequence information. A sequence in FASTA format begins with a single description line, followed by one or more lines of sequence data.

Therefore, a FASTA file has 2 kind of records:

- records which begins with ">", which is a description line (should be ignored for DNA base count)
- records which does not begin with ">", which is a DNA string

We will ignore the description records and focus only on DNA strings.

Example of two FASTA-formatted sequences in a file:

Note that for all three solutions, we will drop description records (which begins with ">" symbol) by using the RDD.filter() transformation.

Solution 1: Classic MapReduce Algorithm

In the canonical example of DNA Base counting, a (key, value) pair is emitted for every DNA base letter found, where key is a DNA base letter in {A, T, C, G} and value is 1 (frequency of one). This solution will create too many (key, value) pairs. After mapping is done, then we have several options for reduction of these (key, value) pairs. The options are:

- Use groupByKey()
- Use reduceByKey()
- Use combineByKey()

Pros of Solution 1

- Simple solution, which works
- Mappers are fast, no need for combining counters

Cons of Solution 1

- Too many (key, value) pairs are created
- Might cause cluster network traffic

Solution 2: In-Mapper-Combiner Algorithm

In this solution we will use In-Mapper-Combiner design pattern and per DNA string, we will emit

at most four (key, value) pairs as:

```
(A, n1)
(T, n2)
(C, n3)
(G, n4)
```

where n1: is the total frequency of A's per mapper input n2: is the total frequency of T's per mapper input n3: is the total frequency of C's per mapper input n4: is the total frequency of G's per mapper input

To implement In-Mapper-Combiner design pattern, we will use Python's <code>collections.Counter()</code> to keep track of DNA base letter frequencies. The other option is to use four variables (initialized to zero), and then increment them as we interate/scan the DNA string. Since the number of keys are very small (4 of them), then it is easier to use 4 variables for counting, otherwise (when you have many keys) you should use a <code>collections.Counter()</code> to keep track of frequencies of keys.

Similar to the first solutions, we mat apply any of the following reducers to find the final DNA base count.

- Use groupByKey()
- Use reduceByKey()
- Use combineByKey()

Pros of Solution 2

- Much less (key, value) pairs are created compared to Solution 1
- In-Mapper-Combiner design pattern is applied
- Will not cause cluster network traffic, since there are not too manny (key, value)

Cons of Solution 2

 A dictionary is created per mapper, if we have too many mappers concurrently, then there might be an OOM error

Solution 3: Mapping Partitions Algorithm

This solution uses [RDD.mapPartitions()] transformation to solve DNA base count problem. In this solution we will emit four (key, value) pairs as:

```
(A, p1)
(T, p2)
(C, p3)
(G, p4)
```

where

```
p1: is the total frequency of A's per single partition
p2: is the total frequency of T's per single partition
p3: is the total frequency of C's per single partition
p4: is the total frequency of G's per single partition
```

Note that a single partition may have thousands or millions of FASTA records. For this solution, we will create a single collections.Counter() per partition (rather than per RDD element)

Pros of Solution 3

- Much less (key, value) pairs are created compared to Solution 1 and 2
- Map Partitions design pattern is applied
- Will not cause cluster network traffic, since there are not too manny (key, value)
- A single dictionary is created per partition. Since the number of partitions can be in hundereds or thousands, this will not be a problem at all
- This is the most scaled-out solution: basically we summarize DNA base counting per partition: from each partition, we emit four (key, value) pairs

Cons of Solution 3

None

Summary and conclusion

In-Mapper-Combiner design pattern is one method to summarize the output of mappers and hence to possibly improve the speed of your MapReduce job by reducing the number of intermediary (key, value) pairs emitted from mappers to reducers. As we noted, there are several ways to implement In-Mapper-Combiner design pattern, which does depend on your mappers input and expected output. One immediate benefit of In-Mapper-Combiner design pattern is to drastically reduce the number of (key, value) pairs emitted from mappers to reducers.

Download FASTA Files

- 1. GeoSymbio Downloads
- 2. NCBI Downloads

3. Filtering Patterns

Filter patterns are a set of design patterns that enables us to filter a set of records (or elements) using different criteria and chaining them in a decoupled way through logical operations. One simple example will be to filter records if the salary of that record is less than 20000. Another example would be to filter records if the record does not contain a valid URL. This type of design pattern comes under structural pattern as this pattern combines multiple criteria to obtain single criteria.

for example, Python offers filtering as:

filter(function, sequence)`

where

function: function that tests if each element of a sequence true or not.

sequence: sequence which needs to be filtered, it can be sets, lists, tuples, or containers of any iterators.

Returns: returns an iterator that is already filtered.

Simple example is given below:

```
# function that filters DNA letters
def is_dna(variable):
    dna_letters = ['A', 'T', 'C', 'G']
    if (variable in dna_letters):
        return True
    else:
        return False
#end-def

# sequence
sequence = ['A', 'B', 'T', 'T', 'C', 'G', 'M', 'R', 'A']

# using filter function
# filtered = ['A', 'T', 'T', 'C', 'G', 'A']
filtered = filter(is_dna, sequence)
```

PySpark offers filtering in large scale for RDDs and DataFrames.

Filter using RDD

Let rdd be an RDD[(String, Integer)]. Assume the goal is to keep (key, value) pairs if and only if the value is greater than 0. It is pretty straightforward to accomplish this in PySpark: by using the RDD.filter() transformation:

```
# rdd: RDD[(String, Integer)]
# filtered: RDD[(key, value)], where value > 0
# e = (key, value)
filtered = rdd.filter(lambda e: e[1] > 0)
```

Also, the filter implementation can be done by boolean predicate functions:

```
def greater_than_zero(e):
    # e = (key, value)
    if e[1] > 0:
        return True
    else:
        return False
#end-def

# filtered: RDD[(key, value)], where value > 0
filtered = rdd.filter(greater_than_zero)
```

Filter using DataFrame

Filtering records using DataFrame can be accomplished by DataFrame.filter() or you may use DataFrame.where().

```
Consider a df as a DataFrame[(emp_id, city, state)].
```

Then you may use the following as filtering patterns:

```
# SparkSession available as 'spark'.
>>> tuples3 = [('e100', 'Cupertino', 'CA'), ('e200', 'Sunnyvale', 'CA'),
            ('e300', 'Troy', 'MI'), ('e400', 'Detroit', 'MI')]
>>> df = spark.createDataFrame(tuples3, ['emp_id', 'city', 'state'])
>>> df.show()
+----+
|emp id| city|state|
+----+
| e100|Cupertino| CA|
| e200|Sunnyvale| CA|
| e300| Troy| MI|
| e400| Detroit| MI|
+----+
>>> df.filter(df.state != "CA").show(truncate=False)
+----+
|emp_id|city |state|
+----+
|e300 |Troy |MI
|e400 |Detroit|MI
+----+
>>> df.filter(df.state == "CA").show(truncate=False)
```

```
+----+
|emp_id|city |state|
+----+
|e100 |Cupertino|CA
|e200 |Sunnyvale|CA
+----+
>>> from pyspark.sql.functions import col
>>> df.filter(col("state") == "MA").show(truncate=False)
+----+
|emp_id|city|state|
+----+
+----+
>>> df.filter(col("state") == "MI").show(truncate=False)
+----+
|emp_id|city |state|
+----+
|e300 |Troy |MI
|e400 |Detroit|MI
+----+
```

You may also use DataFrame.where() function to filter rows:

```
>>> df.where(df.state == 'CA').show()
+----+
|emp_id| city|state|
+----+
| e100|Cupertino| CA|
| e200|Sunnyvale| CA|
+----+
```

For more examples, you may read <u>PySpark Where Filter Function I Multiple Conditions</u>.

4. Organization Patterns

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5. Join Patterns

6. Meta Patterns

Meta data is about a set of data that describes and gives information about other data. Meta patterns is about "patterns that deal with patterns". The term meta patterns is directly translated to "patterns about patterns." For example in MapReduce paradigm, "job chaining" is a meta pattern, which is piecing together several patterns to solve complex data problems. In MapReduce paradigm, another met pattern is "job merging", which is an optimization for performing several data analytics in the same MapReduce job, effectively executing multiple MapReduce jobs with one job.

Spark is a superset of MapReduce paradiagm and deals with meta patterns in terms of estimators, transformers and pipelines, which are discussed here:

- ML Pipelines
- Want to Build Machine Learning Pipelines?

7. Input/Output Patterns

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8. References

- 1. Spark with Python (PySpark) Tutorial For Beginners
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- 5. PySpark Tutorial, author: Mahmoud Parsian
- 6. J. Lin and C. Dyer. Data-Intensive Text Processing with MapReduce