

Max-Minhash Clustering Algorithm of RNA sequences

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Hashing

Hashing functions are an integral part of minwise hashing, as it uses the values of hashing functions to determine similarity between two sets. Therefore, it is necessary that we have a small insight into universal hash functions before moving on to minwise hashing in the next section.

Introduction to hash functions

Imagine a universe of keys $U = \{u_0, u_1, \dots, u_{n-1}\}$ and a range $[r] = \{0, 1, \dots, m-1\}$. Given a hash function $h : U \rightarrow [r]$ which takes any $u_i, i = 0, 1, \dots, n-1$ as argument, it should hold that $\forall u_i, \exists r_j \in [r]$ such that $h(u_i) = r_j$. What remains is to consider collisions, which we define as

$$\delta_h(x, y) = \begin{cases} 1 & \text{if } x \neq y \text{ and } h(x) = h(y) \\ 0 & \text{else} \end{cases} \quad (1)$$

for a given hashfunction h and two keys x and y . The goal of a hashing algorithm is then to minimize the number of collisions across all possible keys. A truly random hash function can assure that there are no collision at all. Unfortunately, to implement such a function would require at least $|U| \log_2 m$ bits[11], defeating the purpose of hash functions altogether. Fixed hashing algorithms have attempted to solve this problem. Unfortunately, its dependence on input causes a worst case average retrieval time of $\Theta(n)$. [4]

Universal hashing can circumvent the memory and computation cost of both random- and fixed hashing, without losing much precision. An introduction to universal hashing will follow, alongside two applications of said hashing which will be tested later in this paper.

Universal hash functions

The first mention of universal hashing was in [3], in which they define universality of hash functions as follows:

Given a class of hash functions $H = \{h : U \rightarrow [r]\}$, H is said to be universal if $\forall x \forall y \in U$

$$\delta_H(x, y) \leq \frac{|H|}{m}$$

where, with $S \subset U$

$$\delta_H(x, S) = \sum_{h \in H} \sum_{y \in S} \delta_h(x, y)$$

That is, H is said to be universal if

$$\Pr_h[h(x) = h(y)] \leq \frac{1}{m} \quad (2)$$

for a random $h \in H$. In many applications, $\Pr_h[h(x) = h(y)] \leq c/m$ for $c = O(1)$ is sufficiently low.

Carter and Wegman[3]

Given a prime $p \geq m$ and a hash function $h_{a,b}^C : [U] \rightarrow [r]$,

$$h_{a,b}^C(x) = ((a * x + b) \mod p) \mod m \quad (3)$$

where a and b are integers mod m , where $a \neq 0$. We want to prove that $h_{a,b}^C(x)$ satisfies Eq. 2; thus proving that it is universal.

Let x and y be two randomly selected keys in U where $x \neq y$. For a given hash function $h_{a,b}^C$,

$$r = a \cdot x + b \mod p$$

$$q = a \cdot y + b \mod p$$

We see that $r \neq q$ since

$$r - q \equiv a(x - y) \mod p$$

must be non-zero since p is prime and both a and $(x - y)$ are non-zero module p , and therefore $a(x - y) > 0$ as two non-zero multiplied by each other cannot be positive, and therefore must also be non-zero module p . Therefore, $\forall a \forall b, h_{a,b}^C$ will map to distinct values for the given x and y , at least at the mod p level.

Dietzfelbinger et al.[6]

Also commonly referred to as **multiply-shift**, this state of the art scheme described in [6] reduces computation time by eliminating the need for the **mod** operator. This is especially useful when the key is larger than 32 bits, in which case Carter and Wegman's suggestion is quite costly[11].

Take a universe $U \geq 2^k$ which is all k -bit numbers. For $l = \{1, \dots, k\}$, the hash functions $h_a^D(x) : \{0, \dots, 2^k - 1\} \rightarrow \{0, \dots, 2^l - 1\}$ are then defined as

$$h_a^D(x) = (a \cdot x \mod 2^k) \div 2^{k-l} \quad (4)$$

for a random odd number $0 < a < 2^k$. l is bitsize of the value the keys map to. The following C-like code shows just how easy the implementation of such an algorithm is

```
h(x)=(unsigned) (a*x) >> (k-l)
```

This scheme only nearly satisfies Eq. 2, as for two distinct $x, y \in U$ and any allowed a

$$\Pr_{h_a^D}[h_a^D(x) = h_a^D(y)] \leq \frac{1}{2^{l-1}} = \frac{2}{m} \quad (5)$$

If Eq. 5 is not sufficiently precise, Wölfel [13, p.18-19] modified this scheme so that it met the requirement in Eq. 2. The hash function is then

$$h_{a,b}^D = ((a \cdot x + b) \mod 2^k) \div 2^{k-l}$$

where $a < 2^k$ is a positive odd number, and $0 \leq b < 2^{k-l}$. This way Eq. 2 is met for $x \neq y \mod 2^k$. For a proof of this, consult [13]¹. The C-like implementation shown below reveals that the modifications are only minimal

```
h(x)=(unsigned)((a*x) + b) >> (k-l)
```

¹The text is in german

Minwise and Maxwise Hashing

Minwise hashing, as described in [2], has repeatedly proven a powerful tool when comparing large sets of strings rapidly, especially for duplicate detection of long articles. The use of minwise hashing for rRNA sequences has already been done in [9], however the method of this paper will be extended by applying two methods of maxwise hashing as described in [7].

Introduction to Minwise Hashing

Let there be two sets A and B . To find the similarity between the two sets, minwise hashing uses is the Jaccard similarity measure, which is defined as

$$J(A, B) = \frac{|A \cap B|}{|A \cup B|} \quad (6)$$

To increase the speed of calculating the Jaccard similarity, it however uses hash functions to find the value. In contrast to calculating the Hamming Distance or the Levenshtein distance², minwise reduces the number of operations needed for the calculation of the Jaccard similarity, by taking advantage of the properties of minwise independent sets[2, pp. 3]. This property will be described below, as well as its application.

Min-wise Independency

Let $H : U \rightarrow [r]$ be a class of hashfunctions. Then for any set $X \subseteq [U]$ and any $x \in X$ and let $h \in H$ be chosen uniformly at random, it is considered minwise independent if

$$\Pr(h_{\min}(X) = h(x)) = \frac{1}{|X|} \quad (7)$$

where

$$h_{\min}(X) = \min\{\forall x \in X, h(x)\}$$

Meaning that all elements in X must have an equal probability of having the minimum value going through h . As seen in Eq. 2, this probability is reachable using universal hash functions.

Min-wise sketch

For two sets A and B it has been proven in [1] that Eq. 7 can be linked to the Jaccard similarity in Eq. 6 as

$$\Pr(h_{\min}(A) = h_{\min}(B)) = \frac{|A \cap B|}{|A \cup B|} \quad (8)$$

For a random set S_1 , we may create a table of random $h_{\min,i}, i = 1, \dots, nh$ such that

$$\hat{S}_1 = \{h_{\min,1}(S_1), h_{\min,2}(S_1), \dots, h_{\min,nh}(S_1)\}$$

²two popular distance metrics that have high precision, but demand long computation time

We may then compute the similarity of two sets \hat{S}_1 and \hat{S}_2 defined by the above equation as

$$J(A, B) = \frac{1}{nh} \cdot \sum_{i=1}^{nh} (h_{\min,i}(S_1) = h_{\min,i}(S_2)) \quad (9)$$

where

$$(h_{\min,i}(S_1) = h_{\min,i}(S_2)) = \begin{cases} 1, & h_{\min,i}(S_1) = h_{\min,i}(S_2) \\ 0, & otherwise \end{cases}$$

which is called the **minwise sketch**. As we see from Eq. 2, there will be a slight error in the calculation of h_{min} . Therefore we must see what influence the size of k will have on the error. A proof of the error using Chernoff Bounds³ is found in [12], shows that the relation between k and ϵ , the error, is

$$k = O\left(\log \frac{1}{\epsilon}\right)$$

Thus, k influences the error inversely exponentially, meaning that $k \approx 100$ should guarantee very small error.

Max-wise hashing

The aforementioned modification is one inspired by the method in the paper [7]. It is an extension of the minwise sketch where in addition to using the min-wise independent sets, we add the maxwise independent set too. Very literally, this means that instead of using the minimum hashvalue, we use the maximal hashvalue such that a set X is said to be maxwise independent if

$$\Pr(h_{\max}(X) = h(x)) = \frac{1}{|X|}, h_{\max} = \max\{\forall x \in X, h(x)\} \quad (10)$$

for any $x \in X$. The Jaccard similarity measure for two sets A and B is

$$\Pr(h_{\max}(A) = h_{\max}(B)) = \frac{|A \cap B|}{|A \cup B|} \quad (11)$$

and finally for a random set S_1 we may create a table of random $h_{\max,i}, i = 1, \dots, k$ such that

$$\tilde{S}_1 = \{h_{\max,1}(S_1), h_{\max,2}(S_1), \dots, h_{\max,k}(S_1)\}$$

This sketch will function almost like the minwise sketch. It is first when combining the two sketches that they have interesting properties.

Combining Max-wise and Min-wise

There are two ways of combining the max-wise and the min-wise algorithm. One is the method in [7], where they halve the amount of hashfunctions, so that for $i = 1, \dots, k/2$

$$J(A, B) = \frac{1}{K} \sum_{i=1}^{K/2} (h_{\min,i}(A) = h_{\min,i}(B) + h_{\max,i}(A) = h_{\max,i}(B)) \quad (12)$$

³A probabilistic method to find the exponentially decreasing bounds between two independent variates.

Let this method be called **Max-minwise halved sketch** (abbr. $\mathbf{Mm}_{\frac{1}{2}}$). This method has been proven to be double as quick as the min-wise hashing, without loss of precision[7]. It is also shown in Lemma 2 in [7] that for $i = 1, \dots, k/2$

$$\Pr(h_{\min,i}(A) = h_{\min,i}(B) | h_{\max,i}(A) = h_{\max,i}(B)) = \frac{|A \cap B| - 1}{|A \cup B| - 1}$$

Meaning that a collision between h_{\min} and h_{\max} is very unlikely.

Another method, which was developed in the course of this paper uses the following combination

$$J(A, B) = \frac{1}{k} \sum_{i=1}^k (h_{\min,i}(A) = h_{\min,i}(B) | h_{\max,i}(A) = h_{\max,i}(B)) \quad (13)$$

where

$$h_{\min,i}(A) = h_{\min,i}(B) | h_{\max,i}(A) = h_{\max,i}(B) = \begin{cases} 1, & h_{\min,i}(S_1) = h_{\min,i}(S_2) \\ 1, & h_{\max,i}(S_1) = h_{\max,i}(S_2) \\ 0, & \text{otherwise} \end{cases}$$

Let this method be called **Max-minwise sketch** (abbr. \mathbf{Mm}). The expected value of \mathbf{Mm} is also the Jaccard similarity by the following proof:

$$\begin{aligned} \frac{1}{k} \sum_{i=1}^k (h_{\min,i}(A) = h_{\min,i}(B) | h_{\max,i}(A) = h_{\max,i}(B)) &= \\ \frac{1}{k} \sum_{i=1}^k (J(A, B) | J(A, B)) &= J(A, B) | J(A, B) = J(A, B) \end{aligned} \quad (14)$$

the final three steps follow from Eq. 9 and Eq. 11. Therefore we see that this method also finds the jaccard similarity.

As one may have noted, the difference between $\mathbf{Mm}_{\frac{1}{2}}$ and \mathbf{Mm} is that the first runs only half as many times as the second for each comparison between two sets.

Additional Tools

A few tools remain to be explained before we can jump into the algorithm. These tools have a variety of reasons for being used that will be explained individually.

k -mer

In order to create the sets that $\mathbf{Mm}_{\frac{1}{2}}$ and \mathbf{Mm} sketches are built with, we shall be using k -mer to partition each sequence into subsets. The k -mer of a sequence string are defined as follows:

The k -mer of a sequence string s is the set of all the substrings of size k of s .

The 1-mer of a sequence string, will therefore be the set of all characters in the sequence string. It is therefore sensible to consider the size of k when partitioning the sequence string.

***k*-mer transformation**

Given that the *k*-mers will be used as hash function input, it is reasonable to transform them to an input that is easy to map. As sequence strings only comprise of 4 characters (A,C,G,T), we assign each character a 2 bit value so that $A = 00, C = 01, G = 10, T/U = 11$, and then put them in sequence according to their position in the substring, eg.

A G T A C
0010110001

which also greatly reduces the memory usage.

MapReduce

Given a sizeable amount of sequences per file, it was quite essential to have a parallel and distributed programming model. For this purpose, MapReduce is a popular programming model. It works by distributing its task to a multitude of workers. Worker can be computers or cores. It expresses its computation as two functions:

1. Map: Runs a function over each element of a list and returns an intermediate value.
2. Reduce: Merges the intermediate values to form a potentially smaller set of values.

As explained in [5], MapReduce processes input by the following steps

1. Map step: Splits the input into M splits. Each split is then distributed to a worker who will perform a Map function on the given split and saves the result into a temporary storage.
2. Shuffle step: The results from the Map calls are then written to a local disk, partitioned into R regions.
3. Reduce step: For each region, a worker is set to run a Reduce job on it, in parallel.

MapReduce has been shown to scale better than other parallel programming tools for input sizes that surpass 100 Mb, which is why it was chosen.[10] Apache Hadoop MapReduce was used, as it is free source.

Pig

Pig Latin is a high level language for compiling and executing MapReduce jobs over Hadoop. Advantageous when performing a pipeline of MapReduce jobs[8], it also demands very few lines of code compared to Hadoop MapReduce code. Additionally, users may write User Defined Functions (abbr. UDF), completely eliminating the need to write any map or reduce function, as they are on the lower level.

Hash Performance Test

Two hashing functions are described in the Hashing section. In order to decide which of these I would use in the algorithm, a few tests were performed in order to determine the speed of each.

To perform these tests, I wrote a short java program. It randomized a given number of k-mer transformations⁴, and then counted the number of nanoseconds it took the Carter Wegman- and multiply-shift hashing schemes to hash all the transformations. The multiply-shift algorithm was set to shift only if the input was longer than 32 bits. In this case, the shift was $2 \cdot k - 32$.

k-mer size	10		20		30	
# of hasvalues	Mult.shift	Carter	Mult.shift	Carter	Mult.shift	Carter
1 mio.	10.3 ± 0.2	11.9 ± 0.5	10.3 ± 0.1	11.6 ± 0.1	10.5 ± 0.1	11.6 ± 0.1
10 mio.	40.9 ± 0.5	42.1 ± 0.2	41.3 ± 0.1	42.1 ± 0.4	41.8 ± 1.6	42.4 ± 0.5
50 mio.	175.5 ± 3.4	187.2 ± 10.6	177.5 ± 2.1	181.6 ± 3.8	176.2 ± 1.3	179.7 ± 1.7
100 mio.	343.0 ± 1.4	377.5 ± 14.0	341.6 ± 1.0	364.1 ± 12.6	346.7 ± 6.9	355.8 ± 3.5

Table 1: *ms* for multiply-shift- and Carter Wegman hashing schemes to 4 different numbers of randomized k-mer transformations.

The results of the tests can be seen in Table 1. The Carter Wegman implementation is consequently smaller than multiply-shift, in addition to having larger margin of error. We may note that the difference in speed is most notable at $k = 10$, diminishing at higher k . It should be noted however that the differences in speed are less than 50 ms, even at 100 mio. input hash values. Also, as the time increases linearly with the number of input values, so will the difference in time.

As the difference in speed is quite minimal, the method used in the algorithm will be the Carter Wegman scheme, as it is easier to implement for input of such different sizes as k-mers.

Implementation

In the following section we will describe how each step of the algorithm is performed in pseudo code. Then, in order to describe the MapReduce flow, we shall explore the Pig script written for the algorithm.

Algorithm

The algorithm will take a few input parameters from the user before running

- a list of sequences $S = s_0, s_1, \dots, s_{N-1}$ of length N
- k -mer size k .
- H , the number of hash functions in the sketch

⁴which are $2 \cdot k$ bits long

- ϵ , the threshold for similarity.

Initially, the sequences had to be transformed into meaningful input for the hash functions used to produce the sketches **MM** and **MM** $_{\frac{1}{2}}$. Natural numbers fit the purpose well, and are exactly what k -mer transformations constitute. The function `kmerTransformation(s, k)`, as seen in Alg. 1, are how the transformations were got. The function `transformChar` uses the same transformation as described in the Tools section.

Algorithm 1 Transforms sequence s into its k -mer transformation

Input: a sequence s , a k -mer size k

Functions: `transformChar(s, k)` maps the characters of a k -mer to 2-bit values, `generateKmer(s, k)` returns the k -mer of s .

Output: The transformed k -mer in a list `kmerTransformed`.

```

1: function KMERTRANSFORMATION( $s, k$ )
2:    $kmer \leftarrow \text{generateKmer}(s, k)$  ▷ saves  $k$ -mer of  $s$ 
3:   for gram in  $kmer$  do
4:      $prod \leftarrow 1$ 
5:      $sum \leftarrow 0$ 
6:     for  $i \leftarrow 0$  to  $gram.length - 1$  do
7:        $sum \leftarrow sum + prod \cdot \text{transformChar}(gram.charAt(i))$ 
8:        $prod \leftarrow prod \cdot 4$ 
9:      $kmerTransformed.append(sum)$ 
10:  return  $kmerTransformed$ 

```

Once the transformations were done, we needed to produce **MM** and **MM** $_{\frac{1}{2}}$. As we concluded in the Hash Performance Test, we were to use the Carter Wegman hash function (Eq. 3), which are referred to as $h_i(x)$ from now on. For the sketch, we generate H hashfunctions for **MM** and $H/2$ hash functions for **MM** $_{\frac{1}{2}}$, each with a different a and b . Alg. 2 shows how **MM** was produced. As we can see, it runs through all H hash functions to find the value that is smallest and highest in the transformed k -mer list. Alg. 3 shows the pseudocode for calculating **MM** $_{\frac{1}{2}}$, where the only change needed was to divide the number of hash functions by two.

The sketches ready, what remained was to compare all sequences' sketches to each other. As speed was a main concern, a greedy algorithm was developed for both **MM** and **MM** $_{\frac{1}{2}}$.

The greed lays in that if the similarity between two sequences is above ϵ , they are immediately placed in the same cluster, regardless of whether there are other clusters that the other sequence is more similar to.

Alg. 4 shows the algorithm for **MM** greedy clustering. In line 1-7 the sketches are prepared for the comparison; the remainder is the greedy algorithm. The most interesting part of this algorithm is line 15-22, where the similarity between two strings is determined. Running through all H hash functions, in line 16-20 it checks that if either $h_{min,i}$ or $h_{max,i}$ of both are equal to the other's counterpart, they are an intersection. When all hash functions have been run

Algorithm 2 Uses transformed k -mer to find **MM** of a sequence

Input: a list of transformed k -mer kT of a sequence, H number of hashfunctions.

Parameters: $h_i(x)$ the i th hash function of the H hash functions initiated.

Output: **MM** of a sequence.

```

1: function TOMMSKETCH( $kT$ )
2:    $MM \leftarrow \emptyset$ 
3:   for  $i \leftarrow 0$  to  $H - 1$  do
4:      $hmin \leftarrow \infty$ 
5:      $hmax \leftarrow -\infty$ 
6:     for  $kt$  in  $kT$  do
7:        $val \leftarrow h_i(kt)$ 
8:       if  $val < hmin$  then  $hmin = val$ 
9:       if  $val > hmax$  then  $hmax = val$ 
10:     $MM.append([hmin, hmax])$ 
11:  return  $kmerTransformed$ 

```

Algorithm 3 Uses transformed k -mer to find **MM** $_{\frac{1}{2}}$ of a sequence

Input: a list of transformed k -mer kT of a sequence, H number of hashfunctions.

Parameters: $h_i(x)$ the i th hash function of the $H/2$ hash functions initiated.

Output: **MM** $_{\frac{1}{2}}$ of a sequence.

```

1: function TOMMSKETCH( $kT$ )
2:    $MMhalf \leftarrow \emptyset$ 
3:   for  $i \leftarrow 0$  to  $H/2 - 1$  do
4:      $hmin \leftarrow \infty$ 
5:      $hmax \leftarrow -\infty$ 
6:     for  $kt$  in  $kT$  do
7:        $val \leftarrow h_i(kt)$ 
8:       if  $val < hmin$  then  $hmin = val$ 
9:       if  $val > hmax$  then  $hmax = val$ 
10:     $MMhalf.append([hmin, hmax])$ 
11:  return  $kmerTransformed$ 

```

through, the similarity between the two strings is determined in line 21. If the similarity then surpasses the given ϵ the strings are placed in the same cluster.

Alg. 5 has a very similar method as Alg. 5. The main difference lies in line 15-22, where the intersections are determined by the number of $h_{min,i}$ that are equal plus the number of $h_{max,i}$ that are equal. This means that each hash function can result in two intersections, instead of one in Alg. 4. Line 20 shows the similarity measure, which is the same as in Alg. 4, since the potential number of intersections was doubled.

Algorithm 4 Greedy Clustering using MM

Input: a list of DNA/RNA sequences $S = \{s_0, s_1, \dots, s_{N-1}\}$ of length N .

Parameters: H number of hash functions, k size of k -mer, ϵ threshold for string similarity, c current cluster

Output: A list of the cluster C each sequence belongs to.

```

1: Initialize  $h_i(x)$  for  $i = 0, 1, \dots, H$ 
2: Initialize  $kT, C$ , and  $MM$  as lists of length  $N$ 
3: for  $i \leftarrow 0$  to  $N - 1$  do
4:    $C[i] \leftarrow 0$ 
5:    $kT[i] \leftarrow \text{kmerTransformation}(s_i)$ 
6:    $MM[i] \leftarrow \text{toMMSketch}(kT[i])$ 
7:  $c \leftarrow 0$ 
8: for  $i \leftarrow 0$  to  $N - 1$  do
9:   if  $C[i] == 0$  then
10:     $c \leftarrow c + 1$ 
11:     $C[i] \leftarrow c$ 
12:    for  $j \leftarrow 0$  to  $N - 1$  do
13:       $intersections \leftarrow 0$ 
14:      if  $C[j] == 0$  then
15:        for  $k \leftarrow 0$  to  $H - 1$  do
16:          if  $MM[i][k][0] == MM[j][k][0]$  then
17:             $intersections \leftarrow intersections + 1$ 
18:          else
19:            if  $MM[i][k][1] == MM[j][k][1]$  then
20:               $intersections \leftarrow intersections + 1$ 
21:          if  $\frac{intersections}{H} \geq \epsilon$  then
22:             $C[j] \leftarrow C[i]$ 

```

Algorithm 5 Greedy Clustering using $\text{MM}_{\frac{1}{2}}$

Input: a list of DNA/RNA sequences $S = \{s_0, s_1, \dots, s_{N-1}\}$ of length N .

Parameters: H number of hash functions, k size of k -mer, ϵ threshold for string similarity, c current cluster

Output: A list of the cluster C each sequence belongs to.

```
1: Initialize  $h_i(x)$  for  $i = 0, 1, \dots, H/2$ 
2: Initialize  $kT, C$ , and  $MM$  as lists of length  $N$ 
3: for  $i \leftarrow 0$  to  $N - 1$  do
4:    $C[i] \leftarrow 0$ 
5:    $kT[i] \leftarrow \text{kmerTransformation}(s_i)$ 
6:    $MM[i] \leftarrow \text{toMMhalfSketch}(kT[i])$ 
7:  $c \leftarrow 0$ 
8: for  $i \leftarrow 0$  to  $N - 1$  do
9:   if  $C[i] == 0$  then
10:     $c \leftarrow c + 1$ 
11:     $C[i] \leftarrow c$ 
12:    for  $j \leftarrow 0$  to  $N - 1$  do
13:       $\text{intersections} \leftarrow 0$ 
14:      if  $C[j] == 0$  then
15:        for  $k \leftarrow 0$  to  $H/2 - 1$  do
16:          if  $MM[i][k][0] == MM[j][k][0]$  then
17:             $\text{intersections} \leftarrow \text{intersections} + 1$ 
18:          if  $MM[i][k][1] == MM[j][k][1]$  then
19:             $\text{intersections} \leftarrow \text{intersections} + 1$ 
20:      if  $\frac{\text{intersections}}{H} \geq \epsilon$  then
21:         $C[j] \leftarrow C[i]$ 
```

MapReduce Flow

Precision Tests

Here are the diagrams for **Mm**

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