Experiments

To access efficiency of both algorithms, and their MapReduce frameworks set of experiements was performed on the data just described. Two different forms of tests were performed; some for measuring the precision of the algorithms, and some for measuring the speed of the algorithms.

For all experiments, $\epsilon = 0.95$. The **MM** clustering algorithm will be refered to as **MM**, likewise will the $\mathbf{MM}\frac{1}{2}$ clustering algorithm be referred to as $\mathbf{MM}\frac{1}{2}$.

Precision tests

In Eq. **??**, a metric of the error was set up for the number of hash functions H. This error did not provide an answer to relation between H and the size of k-mers k and its error. Therefore, a practical testing of this relation was performed, to investigae the precision of **MM** and $\mathbf{MM}\frac{1}{2}$.

A gold standard was instrumental to determine the precision of our algorithms. For this purpose, the Levenshtein similarity was used, as defined in the Tools section. If two strings had a Levenshtein similarity above ϵ they were placed in the same cluster. The gold standard, **GS**, were then set to be the number of clusters found by the Levenshtein similarity clustering algorithm. Once the **GS** were retrieved, the error of an algorithms' found number of clusters, C, could be defined as the difference between C and the gold standard **GS**

$$E = |C - \mathbf{GS}|$$

similarly, the percentage of error E_p was

$$E_p = \frac{|C - \mathbf{GS}|}{\mathbf{GS}}$$

The lower E was, the more precise the algorithm. As both **MM** and $\mathbf{MM}\frac{1}{2}$ results depend on k and H, a large set of tests were performed to determine the precision of each algorithm at many k and H. When the optimal settings were found, the results could then be compared to `uClust` algorithm's precision.

MM precision tests

First, the **MM** algorithm's precision tests were made. In order to narrow down the number of k and H to test, a heat plot of a wide set of k and H for seeing the big scope was made, as seen in Fig. **??**. From this wide study, ostensibly the error increased rapidly at $k > 13$, and $k < 5$ were less precise than $k = 5$. Also, at $H > 80$ the error seemed to stop changing significantly.

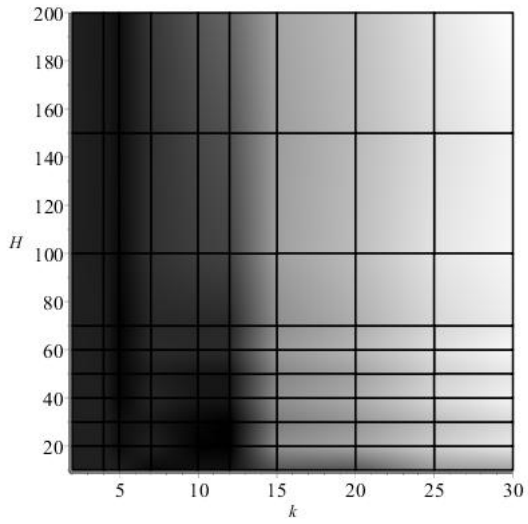


Figure 1: Heat map of the error of **MM** at a widely dispersed array of k and H, run on `Cecum1`. Darkness increases as the error decreases.

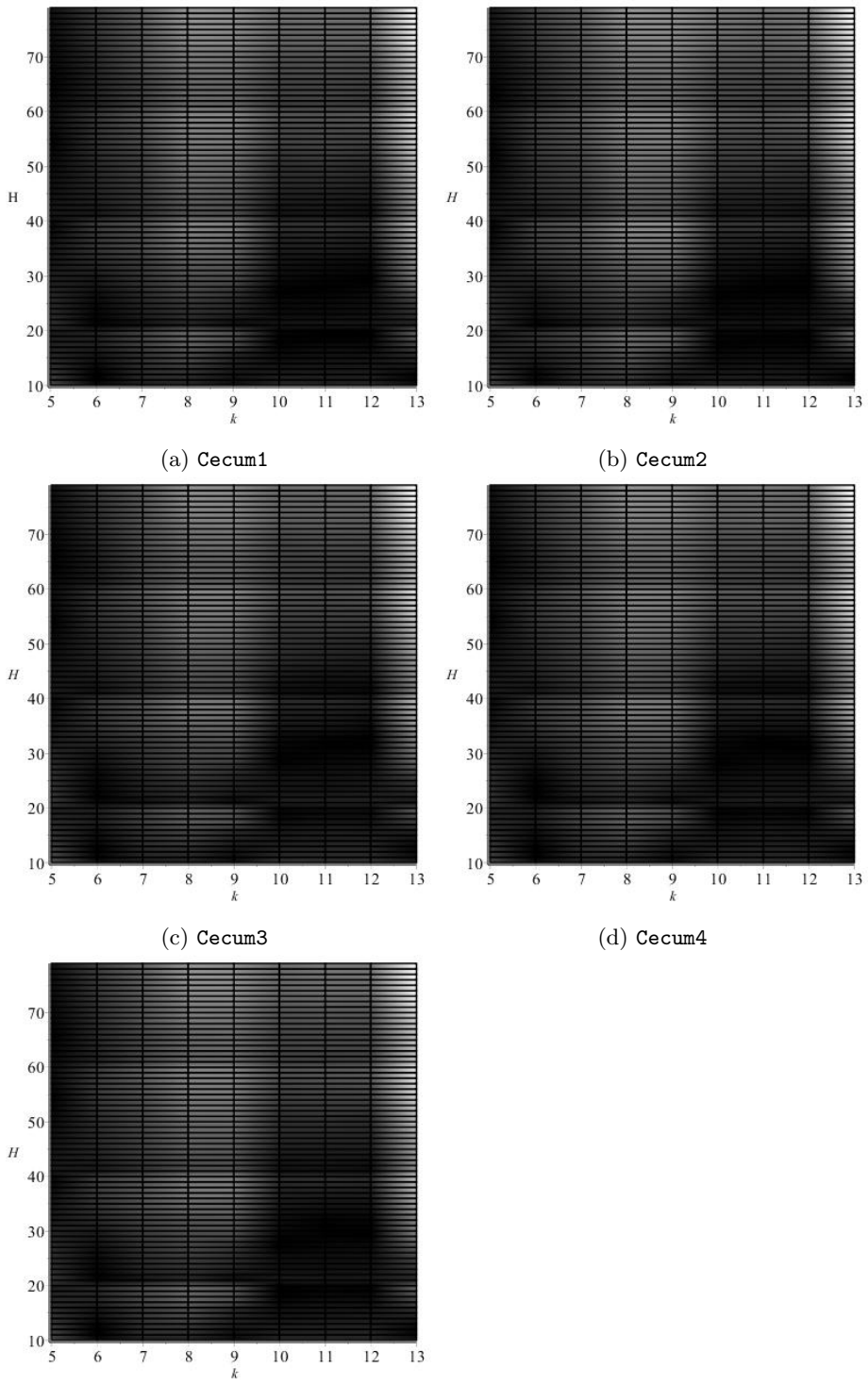
The results of this test showed that the more rigourous tests could be performed at a more narrow set of k and H, as seen in Fig. 2. All heat maps showed very similar results for all samples. There were specific areas that seemed to have repeatedly have a very low error, specifically at

- k=5, a black line from $H = 50$ to $H = 80$.
- $k = 6$, two black spots at around $H = 10$ and $H = 22$.
- $k = 10, 11, 12$, two big black spots at around $H = 16$ and $H = 30$.

These areas of interest were deemed to be most precise. Therefore, each was tested alongside `uClust`, to be able to compare them to each other. Fig. 3 shows the results of these tests.

Fig. 3(a) shows that at $k = 5$, the overall performace of the algorithm appeared near comparable to `uClust`, with a maximum error of approx. 33%. At the spikes, the precision is even higher than `uClust`, most notably at $H = 54$, $H = 65$ and $H = 66$, where the average error over all samples was around 4%. Fig. 3(b) shows that at $k = 6$, the maximal error is around 70%, much worse than that of `uClust`. However, two spikes also appeared here at $H = 13$ and $H = 22$, both with an average error of around 7%, slightly better than `uClust`.

Fig. 3(c-e) show that in spite of generally portraying a high error overall at $k = 10, 11, 12$, reaching maximum errors of over 80%, they still had potentially low errors; Most notably at $k = 10, H = 20$, $k = 11, H = 30$, and $k = 12, H = 30$, with spikes with an average error about 10%, about the same as `uClust`.



(a) `Cecum1`

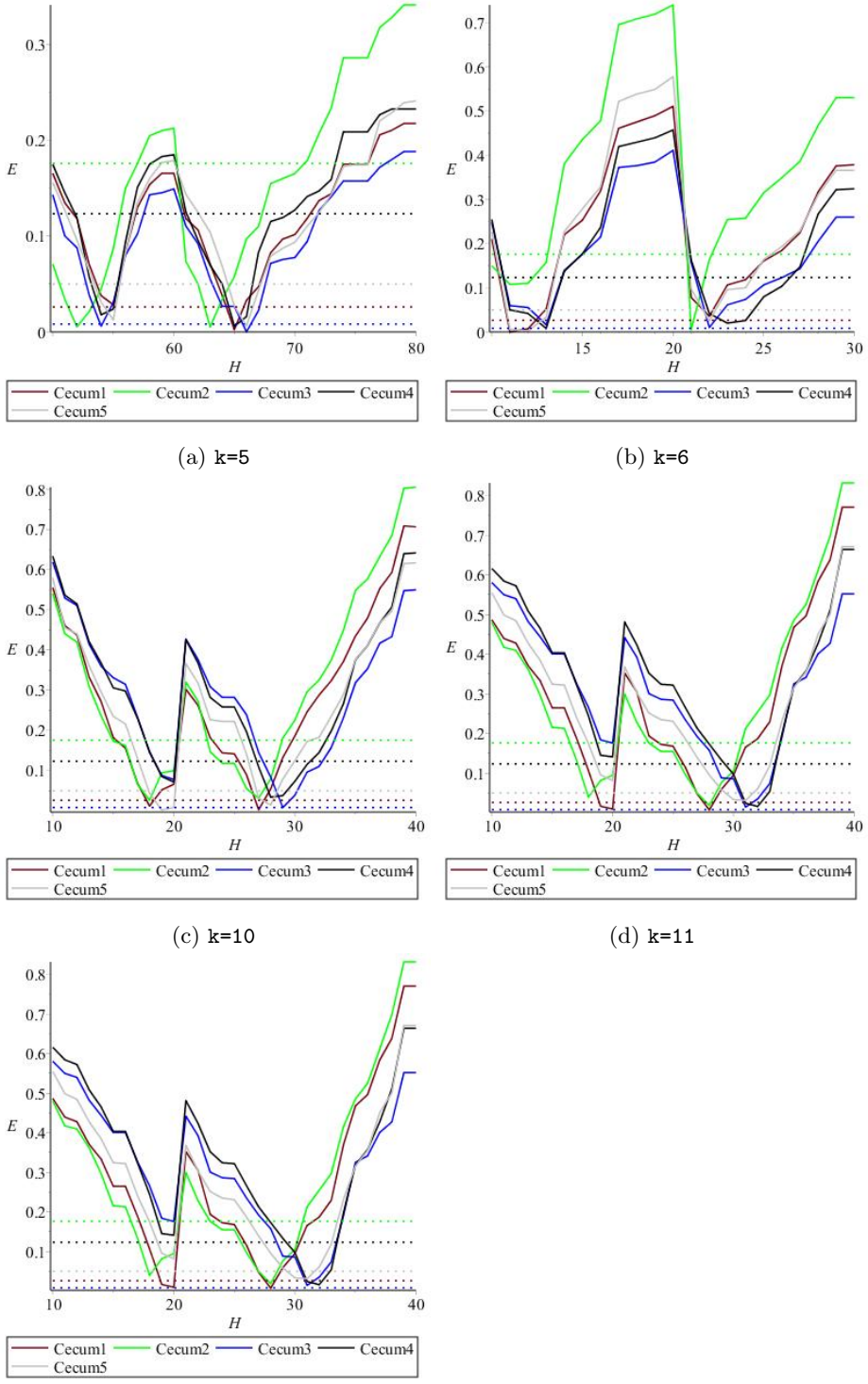
(b) `Cecum2`

(c) `Cecum3`

(d) `Cecum4`

(e) `Cecum5`

Figure 2: Heat maps of the error of **MM** at a narrow array of k and H at all 5 samples of `Cecum` DNA. Darkness increases as the error decreases.



(a) `k=5` (b) `k=6`

(c) `k=10` (d) `k=11`

(e) `k=10`

Figure 3: Plots with H on the x-axis and error E_p in percent ($0.5 = 50\%$) the y-axis, each plot at different k. The lines in the plots signify the error at the given k and H of **MM**, while the dotted lines signify the error of `uClust` at each file. The colours define the sample file.

$\mathbf{MM}^{\frac{1}{2}}$ precision tests

The tests of $\mathbf{MM}^{\frac{1}{2}}$ were performed completely parallel to those of **MM**, but with lower H as reputedly $\mathbf{MM}^{\frac{1}{2}}$ only needs half as many hash functions as the minwise sketch[1]. In Fig. 4 figures the test of a wide array of k and H.

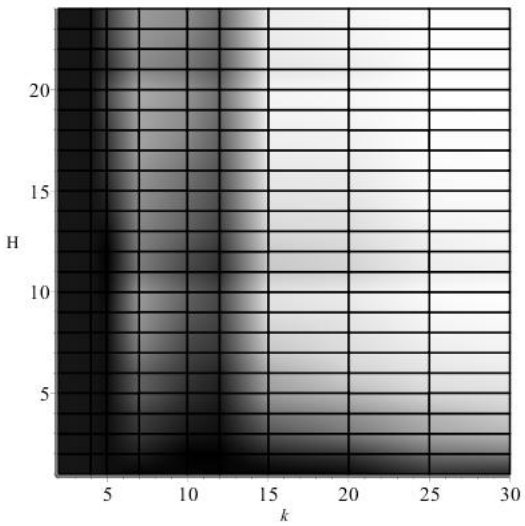


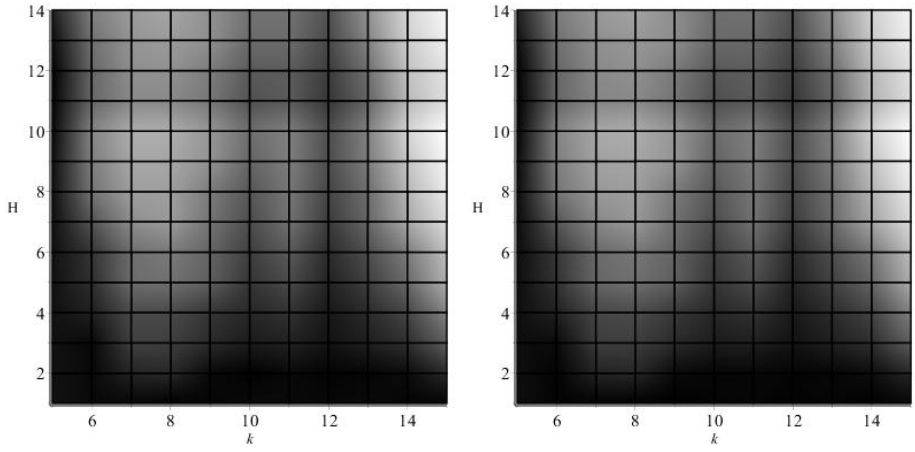
Figure 4: Heat map of the error of $\mathbf{MM}^{\frac{1}{2}}$ at a widely dispersed array of k and H, run on `Cecum1`. Darkness increases as the error decreases.

The large white plateau in Fig. 4 meant that $k > 15$ could be ignored, as the error at this area was very high. Similarly, $k < 5$ gave more error than $k = 5$ and could therefore be ignored. H could be reduced to $H < 15$, as the blackest spot seems around $k = 5, H = 12$.

New tests were performed with these limitations. The results can be seen in Fig. 5. All five plot are almost completely identical, showing that mostly at $H = 1$ and $H = 2$, the precision is highest. The only exception was at $k = 5$, where there seemes to be a lower error along all H. An additional analysis showed that the minimum error in each heat map of Fig. 5 was always at $k = 8, H = 1$. This result was but a stroke of luck, since a single hash function would theoretically cause the error of the $\mathbf{MM}^{\frac{1}{2}}$ sketch to be too high to be applicable for proper comparison (see Eq. **??**).

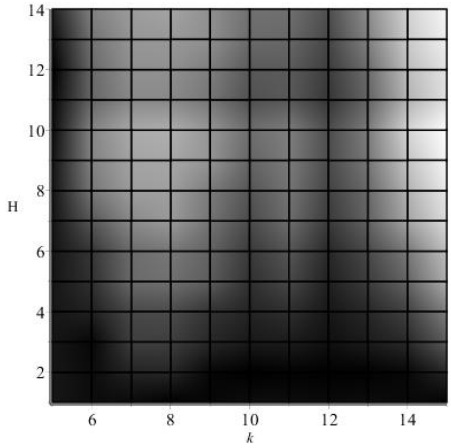
For further analysis of the k of interest, the errors of each file at $k = 5$,$k = 8$ and $k = 12$ were plotted, as seen in Fig. 6. Fig. 6(a-c) all have maximum errors that surpass 100%, even reaching as high as 700% error. Only in Fig. 6(a) a cuspidate spike was present at $H = 12$ with an average error of 20%, around the double of `uClust` average error.

[1] see Minwise and Maxwise Hashing Section

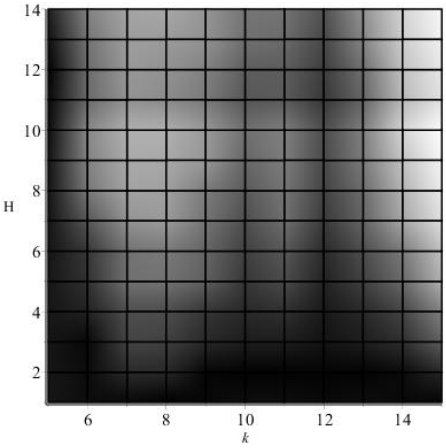


(a) `Cecum1`

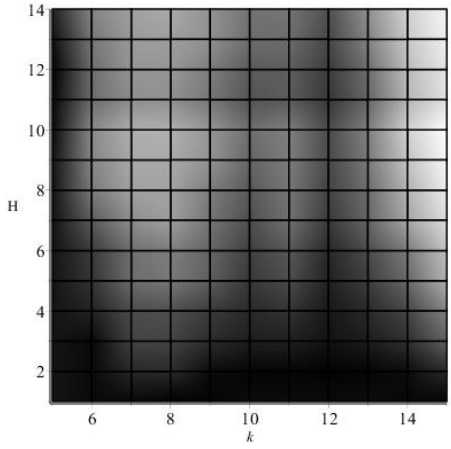
(b) `Cecum2`



(c) `Cecum3`

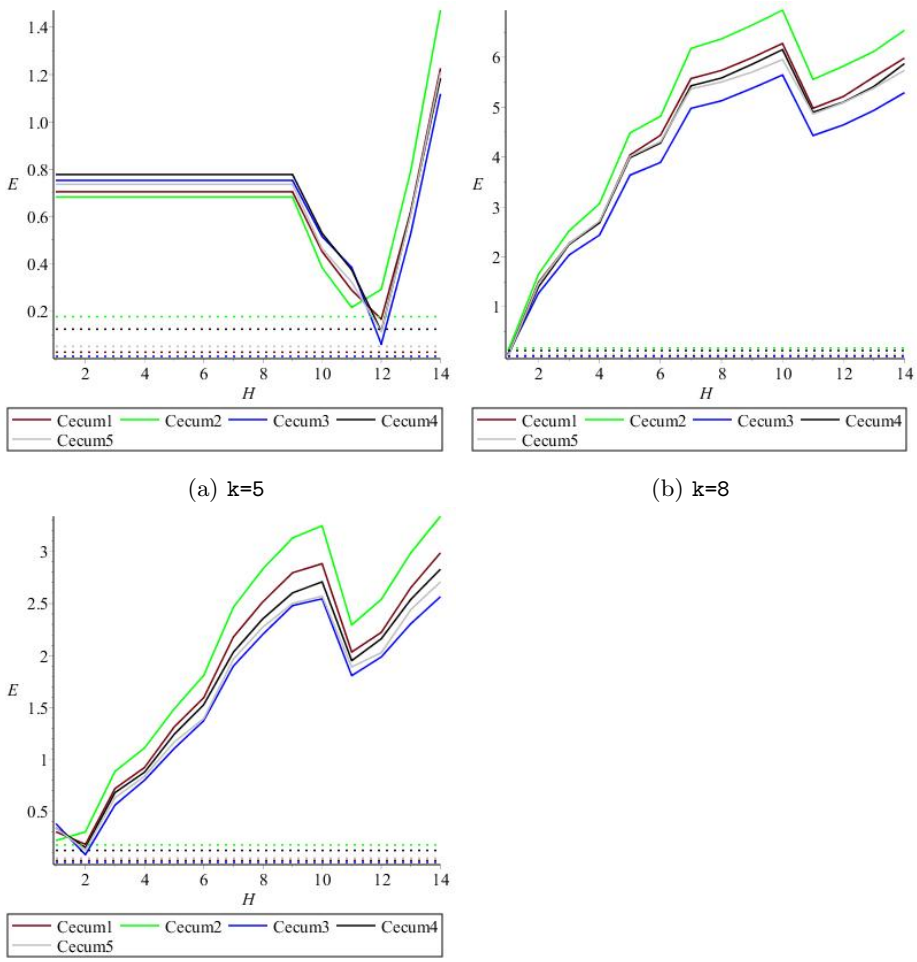


(d) `Cecum4`



(e) `Cecum5`

Figure 5: Heat maps of the error of $\mathbf{MM}\frac{1}{2}$ at a narrow array of k and H at all 5 samples of `Cecum` DNA. Darkness increases as the error decreases



(a) `k=5` (b) `k=8`

(c) `k=12`

Figure 6: Plots with H on the x-axis and error E_p in percent ($0.5 = 50\%$) on the y-axis, each plot at different k. The lines in the plots signify the error at the given k and H of $\mathbf{MM}\frac{1}{2}$, while the dotted lines signify the error of `uClust` at each file. The colours define the sample file.

Comparison

To determine the precision of **MM**, $\mathbf{MM}\frac{1}{2}$ and `uClust`, Fig. 6 and Fig. 3 were perfect candidates. One of the most notable differences between the two graphs was the structure of the results for **MM**, which took an almost "W" like form. The reason for this is from how the sketches of two sequences are compared in Eq. **??**. In contrast to Eq. **??**, **MM** takes advantage of the strong points of both the max- and minwise hashing by finding the intersection of jaccards. This means that if the maxwise hashing is most precise at $H = 12$, and minwise is most precise at $H = 23$, the spikes will appear at these two spots.

Comparing the two, **MM** was quite simply much more precise than $\mathbf{MM}\frac{1}{2}$, by

very large margin. In fact, at the most precise, $\mathbf{MM}^{\frac{1}{2}}$ at $k = 5$ was still not as good as the worst **MM** was at $k = 5$ in our tests. In fact, **MM** turned out to be even more precise than `uClust` at some very specific parameter settings of k and H.

The extreme imprecision of $\mathbf{MM}^{\frac{1}{2}}$ was in fact so high, that it proved almost nonfunctional for practical purposes, if precision in any way was considered of any importance. **MM** however proved that it could compete with `uClust` in terms of precision. Therefore, **MM** was considered a good candidate for an alternative to `uClust`. What remained was to determine whether it could compare speed-wise.

Speed tests

For testing the speed, the MapReduce Framework using Pig Scripts were taken in use for **MM** and $\mathbf{MM}^{\frac{1}{2}}$. `uClust` was run with the setting: `cluster_fast input -id 0.95 -uc output` as storing is also included in the Pig Scripts. As only the 32 bit version of `uClust` was available, there was a memory limit to the size of the operation. For this reason, some of the sample files could not be finished by `uClust`; this occurence will be noted as Mem. Exed.

To achieve the highest speed without loss of too much precision, the precision tests were used to determine the optimal parameters. **MM** was run at $k = 6$ and $H = 13$, which as seen in Fig. 3(b) is comparable to `uClust` in terms of precision. $\mathbf{MM}^{\frac{1}{2}}$ was run with $k = 5$ and $H = 12$.

The results of the test can be seen in Table 1. As expected, $\mathbf{MM}^{\frac{1}{2}}$ was consequently faster than **MM**. Theoretically, $\mathbf{MM}^{\frac{1}{2}}$ should be twice as fast as **MM**. This turned out true in all cases except for the runtime of `Actino1mio` and `Actino500K`. Here $\mathbf{MM}^{\frac{1}{2}}$ was 10 times faster than **MM**, caused by the fact that fewer clusters were produced by $\mathbf{MM}^{\frac{1}{2}}$. Therefore the outer loop of the $\mathbf{MM}^{\frac{1}{2}}$ greedy algorithm iterated less times than the outer loop of **MM**. Such a difference in speed was not predicted, but says more about the imprecision of $\mathbf{MM}^{\frac{1}{2}}$ than the algorithms' relative speed.

The reason why `uClust` was faster in both `Silva50K` and `Actino50K` laid in that the MapReduce Framework had a long startup time[2]. If we had used a single node version of **MM** and $\mathbf{MM}^{\frac{1}{2}}$, we could probably have achieved much higher speeds at samples sizes of 50000 and less, since it would have no startup time. The MapReduce Framework would therefore first be advantageous to a single node solution using input files with 100.000 sequences or more.

Overall, there was a duality of speed between the two sample sets. In the `Actino` sample set, `uClust` consistently ran faster than both **MM** and $\mathbf{MM}^{\frac{1}{2}}$, with an increasing difference in speed over sample size. In the `Silva` samples, both **MM** and $\mathbf{MM}^{\frac{1}{2}}$ ran faster than `uClust` at sample size higher than `Silva50K`. In fact, **MM** was almost twice as fast as `uClust` on the run of `Silva500K`, and the difference in speed increased with sample size.

[2] see section about MapReduce

While the frequency of cases where **MM** and **MM**$\frac{1}{2}$ are faster than `uClust` remains unknown, occasionally **MM** and **MM**$\frac{1}{2}$ trumps `uClust`. In choosing between **MM**$\frac{1}{2}$ and **MM**, a strong case could be made for **MM**. **MM**$\frac{1}{2}$ may have been double as quick as **MM**, but this at the cost of precision. So much precision, that one goes from statistically useless using **MM**$\frac{1}{2}$ to competing with `uClust` using **MM**. And since **MM** was also quicker than `uClust` in some cases, the results suggest that it could serve as a good alternative to `uClust`.

	runtime of sample in s		
Sample	**uClust**	**MM**	**MM**$\frac{1}{2}$
`Actino50K`	2.0	18.3	13.6
`Actino100K`	5.0	23.2	18.7
`Actino200K`	9.0	53.4	28.8
`Actino500K`	14.0	208.4	58.3
`Actino1mio`	Mem. Excd.	1033.8	103.3
`Silva50K`	16.0	18.3	13.6
`Silva100K`	33.0	28.3	18.3
`Silva200K`	70.0	48.6	33.5
`Silva500K`	208.0	133.5	68.3
`Silva1mio`	Mem. Excd.	273.9	128.5

Table 1: Comparison of clustering speed of three algorithms on 10 samples. `uClust` is run with `cluster_fast` option, **MM** with $k = 6$ and $H = 13$, **MM**$\frac{1}{2}$ has $k = 5$ and $H = 12$. The runtime the clustering speed is given in seconds.