Sketching String Similarity

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Outline

Problem Background

My Algorithm for Weighted Jaccard Similarity Estimation

Some other interesting algorithms

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Why do we care?

- Applications: search engine, DNA sequencing, intrusion detection, plagiarism detection etc.

Similarity Measurement

- $S \in \Sigma^*$: string. k-mers of S: substrings of length k.
  e.g.: AATT, TTCC are 4-mers of AATTCCGG.
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- Given 2 sets A, B, the Jaccard Index $J(A,B) = \dfrac{|A \cap B|}{|A \cup B|}$.
- $J_k(S_1, S_2) :=$ Jaccard Index of k-mer sets.
- Recall: MinHash Sketching estimate $J_k(S_1, S_2)$.

Limitation to Jaccard Similarity

By treating S_1, S_2 as sets of k-mers and use $J_k(S_1, S_2)$, we ignore:

- k-mer frequency.
- order in which k-mers appear.

Both factors can affect string similarity.

Limitation to Jaccard Similarity

e.g.: consider:
$S_1 = 000000000000\textcolor{red}{1}00000000000000000000$
$S_2 = 000000000000000000000000000000000$

- Intuitively: S_1, S_2 should be pertty similar (1 character difference.)

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- Intuitively: S_1, S_2 should be pertty similar (1 character difference.)
- But $J_k(S_1, S_2) = \dfrac{1}{k+1} \leq 0.5$.

Limitation to Jaccard Similarity

$S_1 = 000000000000{\color{red}1}00000000000000000000$
$S_2 = 000000000000000000000000000000000$

Idea: even though the "1" in S_1 created k extra k-mers, they should not affect the similarity too much because each of them only appeared once.

Account for frequency!

Limitation of Jaccard Similarity

Might want better measurement of similarity.

- Classical: editing distance.
- We will use a simpler method that extends $J_k(S_1, S_2)$.

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$$J_k^w(S_1, S_2) := \frac{\sum_\sigma \min\{N_k(\sigma, S_1), N_k(\sigma, S_2)\}}{\sum_\sigma \max\{N_k(\sigma, S_1), N_k(\sigma, S_2)\}}$$

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- If ATCG appears 10 times in S_1 and 4 times in S_2, treat the first 4 occurences as "the same".

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e.g.:
$S_1 =$AAAAAAT
$S_2 =$AAAAAT

The 4-mers are $\sigma =$ AAAA and $\tau =$ AAAT.

$$N_4(\sigma,S_1)=3, N_4(\sigma,S_2)=2, N_4(\tau,S_1)=N_4(\tau,S_2)=1$$

So

$$J_4^w(S_1,S_2)=\frac{2+1}{3+1}=\frac{3}{4}=0.75$$

In comparison, $J_4(S_1,S_2)=1$. So the Weighted Jaccard Similarity picks up the difference that S_1 has 1 additional A compared to S_2.

Weighted Jaccard Similarity

$J_k^w(S_1, S_2)$ extends $J_k(S_1, S_2)$?

- Append to each k-mer σ at certain position its occurrence number i: $i =$ the number of times σ appears in S so far.

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If we let $T_k(S)$ denote the set of indexed k-mers of S, then

$$J_k^w(S_1, S_2) = J(T_k(S_1), T_k(S_2)) = \frac{|T_k(S_1) \cap T_k(S_2)|}{|T_k(S_1) \cup T_k(S_2)|}$$

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e.g.: $S_1 =$AAAAAA
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$T_4(S_1) = \{$(AAAA, 1), (AAAA, 2), (AAAA, 3)$\}$
$T_4(S_2) = \{$(AAAA,1)$\}$.

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$$J_4^w(S_1, S_2) = \frac{1}{3} = \frac{|\{(AAAA, 1)\}|}{|\{(AAAA, 1), (AAAA, 2), (AAAA, 3)\}|}.$$

Compute Weighted Jaccard Similarity

Although $J_k^w(S_1, S_2) = J(T_k(S_1), T_k(S_2))$:

- can't simply run MinHash to compute J_k^w if we don't know $T_k(S_1), T_k(S_2)$.
- Brute force: store all their k-mer frequencies and compute $J_k^w(S_1, S_2)$ exactly.
- Low memory?

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MinHash: construct an event (collision of minimum hash values in S_1, S_2) whose probability is $J_k(S_1, S_2)$, the quantity MinHash tries to estimate.

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I wanted to follow the same idea. The goal is to estimate

$$J_k^w(S_1, S_2) = \frac{\sum_\sigma \min\{N_k(\sigma, S_1), N_k(\sigma, S_2)\}}{\sum_\sigma \max\{N_k(\sigma, S_1), N_k(\sigma, S_2)\}} = \frac{|T_k(S_1) \cap T_k(S_2)|}{|T_k(S_1) \cup T_k(S_2)|}$$

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Sample (σ, i) is in $T_k(S_1) \cap T_k(S_2) \iff i \leq \min\{N_k(\sigma, S_1), N_k(\sigma, S_2)\}$, the smaller frequency.

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Problem: don't know $T_k(S_1), T_k(S_2)$ a priori

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Available sample space: all copies of k-mers treated distinct. size = $\sum_{\tau} N_k(\tau, S_1) + N_k(\tau, S_2)$ vs

hope: $T_k(S_1) \cup T_k(S_2)$, size $= \sum_{\tau} \max\{N_k(\tau, S_1), N_k(\tau, S_2)\}$.

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- Maybe: can sample from larger space. Compensate later.

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Turns out, $\mathbb{P}$ can be transformed into $J_k^w(S_1, S_2)$!

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   Next: Check if $(\sigma, m) \in T_k(S) \cap T_k(S')$
4. Pass through S', check if σ appears at least m times in S'. Return 1 if true, 0 otherwise.

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Example:

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sample: (ATTC, 1) in $T_4(S_1)$.

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sample: (ATTC, 1) in $T_4(S_1)$.

Clearly: (ATTC, 1) is also in $T_4(S_2)$. So $f(S_1, S_2, 4)$ returns 1.

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Analysis of p:

Let σ be any k-mer and suppose S_1, S_2 look like:

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$$S_2 = \sigma \ldots \sigma \ldots \sigma \ldots \sigma \ldots$$

where σ and σ mark the last copy of σ in S_1, S_2, respectively. Then by definition, σ is the $N_k(\sigma, S_2)$th copy of σ in S_2. Let σ be the $N_k(\sigma, S_2)$th copy of σ in S_1.

f Explained

Sample = σ and f returns 1 happens in this region:

$$\begin{aligned} S_1 &= \sigma \dots \sigma \dots \sigma \dots \sigma \dots \sigma \dots \\ S_2 &= \sigma \dots \sigma \dots \sigma \dots \sigma \dots \end{aligned}$$

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The circled region above contains
$2 \cdot N_k(\sigma, S_2) = 2 \min\{N_k(\sigma, S_1), N_k(\sigma, S_2)\}$ copies of σ.

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Because of uniform sampling:

$$\mathbb{P}[f \text{ returns 1 and sample is } \sigma] = \frac{2 \min\{N_k(\sigma, S_1), N_k(\sigma, S_2)\}}{\sum_\tau N_k(\tau, S_1) + N_k(\tau, S_2)}$$

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Thus:

$$p = \mathbb{P}[f \text{ returns 1}] = \frac{2\sum_\tau \min\{N_k(\tau, S_1), N_k(\tau, S_2)\}}{\sum_\tau N_k(\tau, S_1) + N_k(\tau, S_2)}$$

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Thus:

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This is not quite what we want:

$$J_k^w(S_1, S_2) = \frac{\sum_\tau \min\{N_k(\tau, S_1), N_k(\tau, S_2)\}}{\sum_\tau \max\{N_k(\tau, S_1), N_k(\tau, S_2)\}}$$

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But, we can write:

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and solve:

$$\frac{p}{2-p} = \frac{\sum_\tau \min\{N_k(\tau, S_1), N_k(\tau, S_2)\}}{\sum_\tau \max\{N_k(\tau, S_1), N_k(\tau, S_2)\}}$$
$$= J_k^w(S_1, S_2)$$

My Algorithm

To estimate $J_k^w(S_1, S_2, k)$, simply run $g(S_1, S_2, k)$:

1. Run R independent copies of $f(S_1, S_2, k)$. $\delta_j =$ return value of the jth copy.
2. $\hat{p} = \frac{1}{R}\sum_{j=1}^{R} \delta_j$.
3. Output $\frac{\hat{p}}{2-\hat{p}}$ as the estimate of $J_k^w(S_1, S_2)$.

In step 1 and 2, $\hat{p} = \frac{1}{R}\sum_{j=1}^{R} \delta_j$ is simply an estimate of the true probability $p = \mathbb{P}[f$ returns 1$]$.

Accuracy Analysis

Because:

- $\mathbb{E}[\hat{p}] = \frac{1}{R}\sum_{j=1}^{R}\mathbb{E}[\delta_j] = p$
- $J_k^w(S_1, S_2) = \frac{p}{2-p}$

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we can hope that $\frac{\hat{p}}{2-\hat{p}}$ will not be too far from $J_k^w(S_1, S_2)$ if $\hat{p}$ is not too far from p.

Accuracy Analysis

Indeed:

$$|\frac{p}{2-p} - \frac{\hat{p}}{2-\hat{p}}| = \frac{2|p-\hat{p}|}{(2-p)(2-\hat{p})} \leq 2|p-\hat{p}|$$

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Simulation: if f is repeated 100 times, then with 0.9 probability, $\frac{\hat{p}}{2-\hat{p}}$ will be within 5 percent of $J_k^w(S_1, S_2)$.

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- Thus: runtime(f) = $O(|S_1| + |S_2|)$, runtime$(g) = O(R(|S_1| + |S_2|))$.
- f only need $O(k)$ space to store k-mer sample and another k-mer in stream.

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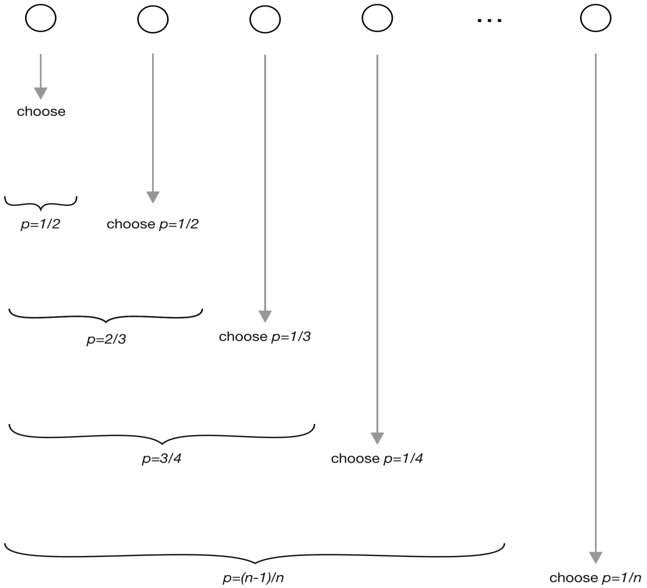
Reservoir Sampling to the rescue.

Streaming Model Considerations

Reservoir Sampling: sample without replacement l items from a stream (unknown length = n).

- We only need to sample 1 item with prob $1/n$.



$$\mathbb{P}[\text{select item } t] = \frac{1}{t} \cdot \frac{t}{t+1} \cdot \frac{t+1}{t+2} \cdots \frac{n-1}{n} = \frac{1}{n}$$

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- f still has runs in $O(|S_1| + |S_2|)$ time and takes $O(k)$ space.
- Need 2 passes in total. Can we do it in one pass? (suspect: no)

Outline

Problem Background

My Algorithm for Weighted Jaccard Similarity Estimation

Some other interesting algorithms

Order MinHash [Marcais, 2019]

Assume access to $T_k(S_1), T_k(S_2)$. (all k-mers are labeled with their occurrence numbers).

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- Estimate (Levenshtein) editing similarity:

$$Ed(S_1, S_2) = \frac{\text{1 - editing distance}}{\max\{|S_1|, |S_2|\}}$$

- Hash functions $\mathcal{H}$: permutations of $T_k(S_1) \cup T_k(S_2)$.

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- Sketch: list of l smallest elements in the order of appearance.
- Collison probability p satisfies:

$$s_1 \le Ed(S_1, S_2) \le s_2 \implies p_1(s_1) \le p \le p_2(s_2)$$

for some $p_1, p_2, s_1, s_2 \in \mathbb{R}$. So by repeated experiments, can estimate p, thus $Ed(S_1, S_2)$.

Order MinHash [Marcais, 2019]

- Editing distance is a very accurate measure.
- But need the stronger assumption about knowing $T_k(S_1), T_k(S_2)$.

HyperLogLog [Flajolet, 2007]

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- Inclusion-exclusion principle: $|A \cap B| = |A| + |B| - |A \cup B|$.
- Can estimate Jaccard index.

HyperLogLog: improvement [Ertl, 2017]

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This is implemented by “Dashing” to produce fast and accurate genome distance estimations.

References

[1] *Locality-sensitive hashing for the edit distance. Marcais, 2019*

[2] *New cardinality estimation algorithms for HyperLogLog sketches. Ertl, 2017*

[3] *HyperLogLog: the analysis of a near-optimal cardinality estimation algorithm. Flajolet, 2007*

[4] *Dashing: fast and accurate genomic distances with HyperLogLog. Baker & Langmead, 2019*