Non-Negative Matrix Factorization Test Cases

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Abstract—Non-negative matrix factorization (NMF) is a problem with many applications, ranging from facial recognition to document clustering. However, due to the variety of algorithms that solve NMF, the randomness involved in these algorithms, and the somewhat subjective nature of the problem, there is no clear “correct answer” to any particular NMF problem, and as a result, it can be hard to test new algorithms. This paper suggests some test cases for NMF algorithms derived from matrices with enumerable exact non-negative factorizations and perturbations of these matrices. Three algorithms using widely divergent approaches to NMF all give similar solutions over these test cases, suggesting that these test cases could be used as test cases for implementations of these existing NMF algorithms as well as potentially new NMF algorithms. This paper also describes how the proposed test cases could be used in practice.

I. INTRODUCTION

What do document clustering, recommender systems, and audio signal processing have in common? All of them are problems that involve finding patterns buried in noisy data. As a result, these three problems are common applications of algorithms that solve non-negative matrix factorization, or NMF [2], [6], [7].

Non-negative matrix factorization involves factoring some matrix $A$, usually large and sparse, into two factors $W$ and $H$, usually of low rank

$$A = WH$$

Because all of the entries in $A$, $W$, and $H$ must be non-negative, and because of the imposition of low rank on $W$ and $H$, an exact factorization rarely exists. Thus NMF algorithms often seek an approximate factorization, where $WH$ is close to $A$. Despite the imprecision, however, the low rank of $W$ and $H$ forces the solution to describe $A$ using fewer parameters, which tends to find underlying patterns in $A$. These underlying patterns are what make NMF of interest to a wide range of applications.

In the decades since NMF was introduced by Seung and Lee [8], a variety of algorithms have been published that compute NMF [9]. However, the non-deterministic nature of these NMF algorithms make them difficult to test. First, NMF asks for approximations rather than exact solutions, so whether or not an output is correct is somewhat subjective. Although cost functions can quantitatively indicate how close a given solution is to being optimal, most algorithms do not claim to find the globally optimal solution, so whether or not an algorithm gives useful solutions can be ambiguous. Secondly, all of the algorithms produced so far are stochastic algorithms, so running the algorithm on the same input multiple times can give different outputs if they use different random number sequences. Thirdly, the algorithms themselves, though often simple to implement, can have very complex behavior that is difficult to understand. As a result, it can be hard to determine whether a proposed algorithm really “solves” NMF.

This paper proposes some test cases that NMF algorithms should solve verifiably. The approach uses very simple input, such as matrices that have exact non-negative factorizations, that reduce the space of possible solutions and ensure that the algorithm finds correct patterns with little noise. In addition, small perturbations of these simple matrices are also used, to ensure that small variations in the matrix $A$ do not drastically change the generated solution.

II. PERTURBATIONS OF ORDER $\epsilon$

Suppose NMF is applied to a non-negative matrix $A$ to get non-negative matrices $W$ and $H$ such that $A \approx WH$. If $A$ is chosen to have an exact non-negative factorization, then the optimal solution satisfies $A = WH$. Furthermore, if $A$ is simple enough, most “good” NMF algorithms will find the exact solution.

For example, suppose $A_0$ is a non-negative square diagonal matrix, and the output $W_0$ and $H_0$ is also specified to be square. Let the diagonal $n \times n$ matrix $A_0$ be denoted $A_0 = \text{diag}(a_0)$, where $a_0$ is an $n$-dimensional vector, so that the diagonal entries $A_0(i,i)$ are $a_0(i)$. It is easy to show that $W_0$ and $H_0$ must be monomial matrices (diagonal matrices under a permutation) [3]. Ignoring the permutation and similarly denoting $W_0 = \text{diag}(w_0)$ and $H_0 = \text{diag}(h_0)$, then $a_0(i) = w_0(i)h_0(i)$ for applicable $i$. Such diagonal matrices $A_0$ were given as input to the known NMF algorithms described in the next section, and all of the algorithms successfully found exact solutions in the form of monomial matrices for $W_0$ and $H_0$.

One way to analyze the properties of an algorithm is to perturb the input by a small amount $\epsilon > 0$ and see how the output changes. Formally, if the input $A_0$ gives output $W_0H_0$, then the output generated from $A_0 + \epsilon A_1$ can be approximated as $(W_0 + \epsilon W_1)(H_0 + \epsilon H_1)$. It is assumed that $\epsilon$ is sufficiently small that $\epsilon^2$ terms are negligible.

For the test case, the nonzero entries of $A_1$ were chosen to be the on the superdiagonal (the first diagonal directly above the main diagonal). This matrix is denoted as $A_1 = $
run with input of the form $A = A_0 + \epsilon A_1$ has $O(1)$ entries on its main diagonal, $O(\epsilon)$ entries on the superdiagonal, and zeroes elsewhere. It is assumed that all the vector entries $a_0(i)$ and $a_1(i)$ are of comparable magnitude.

III. RESULTS FROM VARIOUS ALGORITHMS

Three published NMF algorithms were implemented and run with input of the form $A = A_0 + \epsilon A_1$ as described above. Algorithm 1 was the multiplicative update algorithm described by Seung and Lee in their groundbreaking paper [5], which was run for $10^6$ iterations in each test. Algorithm 2 was the ALS algorithm described in [1], and which was run for $10^6$ iterations as well. Algorithm 3 was a gradient descent method as described by Guan and Tao [4], and was run for $10^4$ iterations. These three algorithms were chosen because they were representative and easy-to-implement algorithms of three distinct types. Many published NMF algorithms are variations of these three algorithms.

The experiments began with the simplest nontrivial case, in which $A$ is a $2 \times 2$ matrix with only three nonzero entries, with fixed $a_0 = [1 \ 1]$ and $a_1 = [1]$, while $\epsilon$ was varied over several different values. Each of the algorithms used randomness in the form of initial seed values for $W$ and $H$. The random seeds were held constant as $\epsilon$ varied. As a result, the outputs from the algorithms with different values of $\epsilon$ were comparable within each test case.

For the $2 \times 2$ case, it is possible to enumerate all of the non-negative exact factorizations of $A$. Given that the factors $W$ and $H$ are also $2 \times 2$ matrices, they can be written as shown below.

$$
\begin{bmatrix}
m & n \\
p & q
\end{bmatrix}
\begin{bmatrix}
r & s \\
t & u
\end{bmatrix} =
\begin{bmatrix}
1 & \epsilon \\
1 & 1
\end{bmatrix}
$$

Multiplying the matrices directly produces the four equations:

$$
\begin{align}
mr + nt &= 1 \\
ms + nu &= \epsilon \\
pr + qt &= 0 \\
ps + qu &= 0
\end{align}
$$

Recall that all entries must be non-negative, so from equation (5), either $p$ or $r$ must be 0, and either $q$ or $t$ must be 0. Furthermore, it cannot be that $p = q = 0$ because that would contradict equation (6), and it cannot be that $r = t = 0$ because that would contradict equation (3). Thus two cases remain: $p = t = 0$ and $q = r = 0$.

Substituting $p = t = 0$ into equations (3), (4), and (6) and solving for $r, s,$ and $u$ gives

$$
r = \frac{1}{m}, \quad s = \frac{1}{m} \left( \epsilon - \frac{n}{q} \right), \quad u = \frac{1}{q}
$$

Likewise, substituting $q = r = 0$ into (3), (4), and (6) and solving for $s, t,$ and $u$ to gives

$$
s = \frac{1}{p}, \quad t = \frac{1}{n}, \quad u = \frac{1}{n} \left( \epsilon - \frac{m}{p} \right)
$$

Observe that these two solutions look similar. In fact, they differ merely by a permutation. In the first case, $W$ and $H$ have the same main diagonal and superdiagonal format as $A$, and can be written in matrix notation as

$$
WH = \begin{bmatrix}
w_0(1) & w_1(1) \\
w_0(2) & w_1(2)
\end{bmatrix}
\begin{bmatrix}
\frac{1}{w_0(1)} & \frac{1}{w_0(1)} (\epsilon - \frac{w_1(1)}{w_0(2)}) \\
\frac{1}{w_0(2)} & \frac{1}{w_0(2)}
\end{bmatrix}
$$

The second case can be written as $(WP)(P^{-1}H)$, where $P$ is the permutation matrix

$$
\begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}
$$

All three of the algorithms tested gave solutions of this form 1000 times out of 1000, for each of several values of $\epsilon$. The consistency of the solutions enabled further analysis. The change in the solution can be measured by the change in the three parameters $w_0(1), w_0(2),$ and $w_1(1)$ (ignoring the permutation if present). Figure 1 shows the change in each of the three parameters from the base case $A_0$ for several different values of $\epsilon$ when input into Algorithm 1. The values of what is the arithmetic mean of the corresponding values generated from 1000 different random seeds. Of course, the precise values depend on the distribution of randomness used. But notice that as $\epsilon$ approaches zero, the values of the three parameters become very nearly linear in $\epsilon$. The results for Algorithms 2 and 3 were very similar - they also showed linearity of the parameters in $\epsilon$, with comparable slopes.

However, $w_1(1)$ was not always linear in $\epsilon$, even for small $\epsilon$. In some cases, the difference approached 0 much more quickly. To see why this occurred, consider that the entries in $H$ could have been chosen to be the parameters rather than the entries in $W$. Also, recall that in the base case $A_0$, in which $\epsilon = 0$, $w_1(1) = h_1(1) = 0$ since both entries are off the diagonal. Thus, when either is linear in $\epsilon$, they are of the form $\epsilon x$ for some slope $x$. Since the solution is exact, it can be deduced that

$$
w_0(1)h_1(1) + w_1(1)h_0(2) = \epsilon
$$
Therefore, in the cases that \( w_1(1) \) approaches 0 very quickly, since \( w_0(1) \) approaches a large, stable value as \( \epsilon \) approaches 0, \( h_1(1) \) must be nearly linear in \( \epsilon \). So in the cases that \( w_1(1) \) is not linear in \( \epsilon \), its symmetrical counterpart, \( h_1(1) \), is. To simplify this complication out of the data, the parameters in \( W \) were chosen when \( w_1(1) \) was closer to linearity in \( \epsilon \), and the parameters in \( H \) were chosen when \( h_1(1) \) was closer to linearity in \( \epsilon \).

Curiously, although it was possible for \( w_1(1) \) and \( h_1(1) \) to “split” the nonlinearity so that both were somewhat linear, this rarely occurred. All three algorithms preferred to make one of them very close to linear at the expense of the other. When \( w_1(1) \) approached zero very rapidly, by equations (3) and (4), \( h_1(1) = c h_0(1) \), and similarly, when \( h_1(1) \) is negligible, \( w_1(1) = c h_0(2) \).

Next, different values for the entries of \( a_0 \) and \( a_1 \) were tried, so they had a range of entries rather than all 1’s. The algorithms all behaved similarly; up to permutation, they satisfied the following formula

\[
W H = \begin{bmatrix}
  w_0(1) & w_1(1) \\
  w_0(2) & w_0(2)
\end{bmatrix} \begin{bmatrix}
  a_0(1) & a_1(1) \\
  a_0(1) & a_0(1) \epsilon - w_1(1)a_0(2) \\
  a_0(2) & a_0(2)
\end{bmatrix}
\]

Note that equation (9) is just a special case of this equation in which \( a_0(1) = a_0(2) = a_1(1) = 1 \). The same phenomena was also observed in which the algorithm usually made one of \( w_1(1) \) and \( h_1(1) \) be nearly linear in \( \epsilon \) and the other approach zero rapidly, rather than having both entries be non-negligible.

As long as the entries of \( a_0 \) and \( a_1 \) are roughly on the order of 1, the algorithms operated similarly.

The next case examined set \( A \) to be a 3 × 3 matrix. Using similar logic to the 2 × 2 case, it can be deduced that any exact factorization of \( A \) is likely to be of the form

\[
\begin{bmatrix}
w_0(1) & w_1(1) & \epsilon w_0(1)h_0(1) \\
w_0(2) & w_1(2) & \epsilon w_0(2)h_0(2) \\
w_0(3) & \epsilon w_0(3)h_0(3)
\end{bmatrix}
\]

Indeed, all three algorithms always gave solutions of this form. In fact, most of the time there were two more zero entries than necessary - either \( w_1(1) \) or \( h_1(1) \), and either \( w_1(2) \) or \( h_1(2) \). This is similar to the way that \( w_1(1) \) or \( h_1(1) \) often approached 0 rapidly in the 2 × 2 case. To note another similarity to the 2 × 2 case, whenever \( w_1(i) \) was significant and \( h_1(i) \) was not, \( w_1(i) \) was very close to \( \epsilon w_0(i + 1) \) - in similar situations \( h_1(i) \) was approximately \( c h_0(i) \).

As a result, there were 4 distinct configurations of the nonzero elements in the solutions, as given by Figure 2. Note that Type IV appears to be an inexact solution; since it has positive \( w_1(1) \) and \( h_1(2) \), the entry at position \( A(1, 3) = w_1(1)h_1(2) \) in the product \( WH \) would have to be nonzero. However, both \( w_1(1) \) and \( h_1(2) \), like all entries on the superdiagonal, are \( O(\epsilon) \), so \( w_1(1)h_1(2) \) is \( O(\epsilon^2) \), and is considered negligible. In fact, most of the solutions generated by the algorithms had nonzero values for entries that were supposed to be zero, but for this analysis anything below \( O(\epsilon^2) \) was considered negligible.
the algorithms are cubic in the size of the matrix, at best, the sample size for large matrices is small.

IV. PROPOSED TESTS FOR NMF ALGORITHMS

Since all three algorithms, which cover a variety of approaches to NMF, had a lot in common in their solutions, it is propose that these inputs $A$ could be used as a test case of an NMF algorithm implementation. In this section, it is proposed how such test cases could be executed.

The test begins with input of the form

$$A = A_0 + \epsilon A_1 = \text{diag}(a_0) + c \text{diag}(a_1, 1)$$  (13)

$A$ is square, and preferably somewhere between $3 \times 3$ and $8 \times 8$ in size, although bigger inputs may be useful as well. The entries should vary between tests. Each test should start by using $\epsilon = 0$ so that $A$ is diagonal. The results of this test should have $W$ and $H$ monomial - only one nonzero element in each row and column. Ignore entries that are below $O(10^{-10})$, for the entirety of testing, as any such entries are negligible.

If $W$ or $H$ is not monomial, or if the product $WH$ is not equal to $A$ to within a negligible margin of error, the algorithm fails the test. Otherwise, the generated solution can be used to find the permutation matrix $P$ that makes $WP$ and $P^{-1}H$ diagonal by replacing the nonzero entries of $H$ with 1's. Since $A = WH$ is diagonal, $WP$ is also diagonal, and since $I = P^{-1}P$ is diagonal, so is $P^{-1}H$. Knowing $P$ will make the rest of the testing much simpler since it is easier to identify whether a solution is of the form given above when it is not permuted.

Next, run the test again using a positive value for $\epsilon$; $\epsilon = 10^{-3}$ seems to work well, although using a variety of $\epsilon$ is also recommended. Make sure to use the same random seeds that were used in the $\epsilon = 0$ test to produce corresponding output. Then check that the $W$ and $H$ given by the algorithm are such that $WP$ and $P^{-1}H$ have nonzero entries only on the two diagonals that they are supposed to. If this doesn’t hold, changing $\epsilon$ might have changed which permutation returns $W$ and $H$ to the proper form, so check again; this happens more commonly among larger matrices than smaller ones. However, if $W$ and $H$ really do break the form, or $A \neq WH$, the algorithm fails the test on this input. Otherwise, it passes.

Note that even widely accepted algorithms do fail these tests occasionally, especially with matrices larger than $8 \times 8$, so it’s advisable to perform the test many times to get a more accurate idea of an algorithm’s performance.

V. CONCLUSION

This paper proposes an approach to the problem of testing NMF algorithms by running the algorithms on simple input that can produce an exact non-negative factorization, and perturbations of such input. In particular, square matrices with $O(1)$ entries on the main diagonal and $O(\epsilon)$ entries on the superdiagonal are proposed, because they have exact solutions that can enumerated mathematically, or because they are perturbations of matrices with exact solutions.

The test cases have been used as input on three known NMF algorithms that represent a variety of algorithms, and all of them behaved similarly, which suggests testable, quantifiable behaviors that many NMF algorithms share. These test cases offer one approach for testing candidate NMF implementations to help determine whether it behaves as it should.

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