NONNEGATIVE MATRIX FACTORIZATION (NMF) WITH HETEROSEDASTIC UNCERTAINTIES AND MISSING DATA

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Abstract

Dimensionality reduction and matrix factorization techniques are important and useful machine-learning techniques in many fields. Nonnegative matrix factorization (NMF) is particularly useful for spectral analysis and image processing in astronomy. I present the vectorized update rules and an independent proof of their convergence for NMF with heteroscedastic measurements and missing data. I release a Python implementation of the rules and use an optical spectroscopic dataset of extragalactic sources as an example for demonstration.

Subject headings: surveys – methods: data analysis – methods: statistical – methods: observational

1. INTRODUCTION

Astronomy has always been at the forefront of intensive data analysis. Among the machine-learning techniques that are commonly used in the field, dimensionality reduction and matrix factorization techniques are particularly useful, as astronomical observations often produce measurements with highly-correlated dimensions. We can extract the most essential physics from the few intrinsic dimensions revealed with the techniques. They also provide a powerful tool for extrapolating the data from current observations and making predictions for future experiments.

The most popular dimensionality reduction technique is probably principal component analysis (PCA). Given a dataset, PCA finds the orthogonal dimensions and ranks them according to their contributions to the sample variance. However, a limitation of the standard PCA is that the sample variance includes both intrinsic variance (among true values of instances) and measurement uncertainties (for a given instance) in real-life applications. In astronomy, a few works have improved upon the standard PCA and developed iterative methods to handle the heteroscedasticity of astronomical data, usually based on the Expectation-Maximization optimization (e.g., Connolly & Szalay 1999; Budavári et al. 2009; Bailey 2012).

An alternative method to PCA is nonnegative matrix factorization (NMF), which restricts the dimensions to the nonnegative half-space. It can be particularly useful in astronomy, since the flux of an object does not go negative (in principle). In their seminal paper, Lee & Seung (2001) introduced simple multiplicative update rules for standard NMF with homoscedastic data. Later, Blanton & Roweis (2007) presented new update rules that can take into account nonuniform uncertainties and missing data. Blondel et al. (2008) presented a vectorized version and a proof following the same methodology as Lee & Seung (2001) for homoscedastic data. I here present an independent study of the vectorized rules and a proof for the convergence of the weight cost function under these rules, by extending the original proof by Lee & Seung (2001). I also provide a summary of the relevant formulas. The vectorized rules are very straightforward to implement in a modern vector language. I here release a Python implementation of the algorithm and use an optical spectroscopic dataset of extragalactic sources as an example for demonstration.

2. NONNEGATIVE MATRIX FACTORIZATION

Nonnegative matrix factorization is, for a given nonnegative matrix $X$, find nonnegative matrix factors $W$ and $H$ such that

$$X \approx WH.$$  \hspace{1cm} (1)

We will assume the dimensions of $X$, $W$ and $H$ are $l \times m$, $l \times n$, and $n \times m$, respectively, where $n$ is a free parameter to be determined by the user. When discussing any given row, column, or element, we will use $i$, $j$, and $k$ to indicate the indices in the dimensions specified by $l$, $m$, and $n$, respectively.

In the PCA language, we often interpret one of the two factors as the set of basis components and the other as the coefficients. In practice, which one is which depends on how one interprets the dimensions of the original data matrix $X$. In addition, a trivial transpose operation shows the symmetry between the two factors:

$$X^T \approx H^T W^T,$$  \hspace{1cm} (2)

and after swapping the rows and columns all the discussions below still apply.

2.1. The update rules for homoscedastic data

To find the two factors $W$ and $H$, as PCA, the goal of NMF is to minimize the least squares error (squared Frobenius norm) as the cost function:

3 I here do not call NMF components eigen-components or eigenvectors, since they are not orthogonal to each other because of the nonnegativity constraint. I also do not label them principal components to avoid confusion with components from PCA, though I note that one can still rank the basis components by their contributions to the variance within the dataset.
\[
\chi^2 = \| (X - WH) \|^2 \\
= \sum_{ij} \left( X_{ij} - \sum_k W_{ik} H_{kj} \right)^2
\]
assuming homoscedasticity of the data.\(^4\)

**Lee & Seung (2001)** showed that this cost function is nonincreasing under the following multiplicative update rules:

\[
H \leftarrow H \odot \frac{W^T X}{W^T WH}, \tag{5}
\]

\[
W \leftarrow W \odot \frac{XH^T}{WHH^T}, \tag{6}
\]

where \(\odot\) represents the element-wise product (the Hadamard product)\(^5\) and \(\div\) the element-wise division.

It is worth pointing out that the above rules for \(H\) and \(W\) are independent of each other, and under each of them (with the other one fixed) the cost function \(\chi^2\) is guaranteed to be nonincreasing, as shown in their seminal paper by **Lee & Seung (2001)**. This means if we are trying to learn the two factors simultaneously, we need to apply them in sequential order, i.e., once we update \(H\), we need to use the new updated \(H\) when updating \(W\) in the next step, and vice versa, although which one goes first does not matter.\(^6\)

As another consequence, a great advantage of these rules is that, if we have known one of the two factors and are only interested in learning the other, we can just use the corresponding rule as a projection mode while simply ignoring the other.

As many other optimization methods, the update rules above can converge to a local minimum and are not guaranteed to yield the optimal solution. In practice, we can generate many different initializations and select the best solution. On the other hand, we can also increase the free parameter \(n\), which is often interpreted as the number of components, and find a better solution that reduces the cost.

### 2.2. The update rules for heteroscedastic data

#### 2.2.1. The update rules

The cost function and update rules above assume homoscedasticity. In astronomy, we often face the challenge with nonuniform uncertainties and missing data. To account for the heteroscedasticity, we therefore should minimize the weighted cost function:

\[
\chi^2 = \| V^{\frac{1}{2}} \odot (X - WH) \|^2 \\
= \sum_{ij} \left( V_{ij}^{\frac{1}{2}} X_{ij} - V_{ij}^{\frac{1}{2}} \sum_k W_{ik} H_{kj} \right)^2
\]

where the weight \(V\) has the same dimension as \(X\) and a common choice is the inverse variance matrix \(1/\sigma^2\), and the square and square root apply element-wise. If we have missing data, we can simply use a binary mask matrix \(M\), in which a 0-valued (False) element indicates a missing datum, and use \(V \odot M\) as the new weight.

To minimize the new weighted cost function, **Blanton & Roweis (2007)** presented new update rules (see A22 and A24 in their appendix), which uses indexed elements explicitly. **Blondel et al. (2008)** presented a vectorized version of the update rules, and also a proof following the same methodology as **Lee & Seung (2001)**. I here present an independent study of the vectorized rules and also provide an alternative proof in the next section, built upon the one by **Lee & Seung (2001)**.

The vectorized update rules are

\[
H \leftarrow H \odot \frac{W^T (V \odot X)}{W^T [V \odot (WH)]}, \tag{9}
\]

\[
W \leftarrow W \odot \frac{(V \odot X) H^T}{[V \odot (WH)] H^T}. \tag{10}
\]

Compared to the original rules (Eq. 5 and Eq. 6), we have simply replaced \(X\) (in the numerators) and \(WH\) (in the denominators) with the weighted versions, \(V \odot X\) and \(V \odot (WH)\). I provide a proof below that under each of these rules the new weighted cost function is nonincreasing.

#### 2.2.2. A Proof

Here provide a proof that under the update rules Eq. 9 and Eq. 10, the weighted cost function Eq. 7 is nonincreasing, assuming the theorems in **Lee & Seung (2001)** hold. I refer the reader to **Blondel et al. (2008)** for a different proof, which includes proving the similar theorems as in **Lee & Seung (2001)**.

We first take a closer look at the original cost function Eq. 3 and the update rules Eq. 5 and Eq. 6. First I note that the update rule Eq. 5 applies to each column without interference (between the columns), i.e., the update rule is equivalent to updating every column \(j\) in \(H\) in parallel:\(^7\)

\[
H_j \leftarrow H_j \odot \frac{W^T X_j}{W^T WH_j}, \tag{11}
\]

and the cost function can be written as a sum of contributions from all the columns:

\[
\chi^2 = \sum_j \| (X_j - WH_j) \|^2 \tag{12}
= \sum_j \chi_{j}^2. \tag{13}
\]

This is the strategy used by **Lee & Seung (2001)**, who provided the proof for the theorem that, the contribution to the cost function from a given column \(j\), \(\chi_{j}^2\), is nonincreasing under the update rule above (Eq. 11), and therefore the sum of the contributions from all the columns, \(\chi^2\), is also nonincreasing. I refer the reader to **Lee & Seung (2001)**.

\(^4\) The Hadamard product is commutative, associative and distributive over addition.

\(^5\) We can update \(H\) (\(W\)) many times before updating \(W\) (\(H\)).

\(^6\) This feature can therefore be used to improve the efficiency of NMF with parallel programming.
their paper for its proof and here I will take it as a theorem, and use it to prove that under the following update rule for a given column $j$,

$$H_j \leftarrow H_j \circ \frac{W^T (V_j \circ X_j)}{W^T [V_j \circ (WH_j)]},$$  

(14)

its contribution to the weighted cost function,

$$\chi_j^2 = \left\| V_j^\circ (X_j - WH_j) \right\|^2,$$  

(15)

is nonincreasing.

To prove this, note that the update rules for $H$ and $W$ are independent of each other and are applied with the other one fixed. When updating $H_j$, we can define $\hat{X}$ and $\hat{W}$:

$$\hat{X}_j \equiv V_j^\circ X_j,$$  

(16)

$$\hat{W} \equiv [V_j^\circ]^\text{diag} W,$$  

(17)

where $[V_j^\circ]^\text{diag}$ represents a diagonal matrix with $V_j^\circ$ as the diagonal elements.

We can now re-write Eq. (15) as

$$\chi_j^2 = \left\| (\hat{X}_j - \hat{W}H_j) \right\|^2.$$  

(18)

And a little algebra shows that the update rule Eq. (14) can be re-written as

$$H_j \leftarrow H_j \circ \frac{W^T \hat{X}_j}{W^T \hat{W}H_j}.$$  

(19)

Now we can apply the original proof by Lee & Seung (2001) and show that, under the rule Eq. (19) the cost Eq. (18) is nonincreasing.

With a simple transpose operation as in Eq. (2) we can also show that under the update rule Eq. (10) the weighted cost function Eq. (7) is nonincreasing. For completeness, alternatively, we can also decompose the cost function into contributions from every row in $X$:

$$\chi^2 = \sum_i \left\| V_i^\circ (X_i - W_iH) \right\|^2$$  

(20)

$$= \sum_i \chi_i^2.$$  

(21)

By defining

$$\hat{X}_i \equiv V_i^\circ X_i,$$  

(22)

$$\hat{H} \equiv H [V_i^\circ]^\text{diag},$$  

(23)

where $[V_i^\circ]^\text{diag}$ represents a diagonal matrix with $V_i^\circ$ as the diagonal elements. we can re-write the update rule Eq. (10) for a given row $i$ as

$$W_i \leftarrow W_i \circ \frac{(V_i \circ X_i) H^T}{[V_i \circ (W_iH)]H^T},$$  

(24)

$$= W_i \circ \frac{\hat{X}_i \hat{H}^T}{W_i \hat{H} H^T},$$  

(25)

under which the contribution to the weighted cost function from row $i$,

$$\chi_i^2 = \left\| (\hat{X}_i - W_i\hat{H}) \right\|^2,$$  

(26)

is nonincreasing.

3. AN EXAMPLE

It is easy to implement the vectorized algorithm above in any vector language. I here release a Python implementation, taking advantage of the fast NumPy package that has BLAS and LAPACK incorporated. I present a brief introduction of the code in the Appendix. Here I use an optical spectroscopic dataset of extragalactic sources as an example to demonstrate how to apply the technique in practice.

3.1. The test dataset

To further illustrate the algorithm, I use an optical spectroscopic dataset of extragalactic sources as an example. This dataset was also used as a test case in Zhu (2016) for classification purposes and can be downloaded on the Web, as shown in the Appendix. I select the sources and their spectra from the seventh data release (DR7, Abazajian et al. 2009) of the Sloan Digital Sky Survey (York et al. 2000). More specifically, I select sources at redshift $z \sim 0.05$ with high-S/N (15–30) spectra. The test dataset includes 2820 extragalactic sources and I consider the wavelength range between 3700 Å and 7000 Å. Although a small sample, this dataset spans a variety of astrophysical sources, including quiescent, star-forming galaxies with different metallicities, AGN, etc., and serves well for the testing purposes.

3.2. The basis sets

I construct basis sets with the number of components $n$ ranging from 2 to 24. For comparison purposes, for a given $n$, I initialize the first $n - 1$ components with the previous basis set, except for the first basis set with $n = 2$, for which I generate random number matrices
Fig. 2.— The basis sets for the extragalactic spectroscopic test dataset, for $n = 3$ to $n = 10$. Note I have skipped the first 5 components for $n = 7$ to $n = 10$, which are similar to the basis set for $n = 5$.

To take a closer look, I show the basis sets for $n = 3$ to $n = 10$ in Figure 2. Note I use the basis set for $n - 1$ as the initial set at the construction for $n$, so the first $n - 1$ components of each basis set are almost the same as the previous basis set. For $n = 7$ to $n = 10$, I have skipped the first 5 components, which are very similar to the basis set for $n = 5$. Looking at the first two components (which form the basis set for $n = 2$), we see a red template that looks like the spectrum of a quiescent galaxy dominated by old stellar populations (see, e.g., Thomas et al. 2005; Zhu et al. 2010) and a blue template that appears to be the spectrum of a star-forming galaxy with strong emission lines (see, e.g., Kennicutt 1992).

with values between 0 and 1 as initial guesses. This way we create a roughly ranked list of basis components based on their contributions to the sample variance. However, I would like to stress that this construction method is devised only for the convenience of comparing the basis sets with different numbers of components. As discussed earlier, the update rules of NMF are not guaranteed to converge to the global minimum of the cost function.

In Figure 1 I show the progression of the reduced $\chi^2_{\text{red}}$, the total cost divided by the data size minus the number of components $n$, as a function of $n$. The cost converges quickly and at $n = 10$, it is already less than 5% higher than at $n = 24$. 

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The third component adds a bluer template that appears to be a combination of B, A and F types of stars. The fourth and the seventh components show variations of stellar absorption features, likely to account for the range of stellar age and metallicity covered by the sample.

The rest of the components mostly include emission lines with varying ratios. This is because in different types of systems, different physical mechanisms are responsible for exciting the atoms/ions, resulting in a variety of emission-line properties. These strong emission lines can account for a considerable fraction of the least squares error and therefore require a number of basis components with varying ratios to cover the variance.

### 3.3. The basis set with partial data

We can handle missing data easily with the algorithm described above, simply by providing a mask $M$. It is interesting to explore the effects of missing data on the modeling. To do so, I randomly select 20\% of the data\footnote{I do not select random objects and exclude their full spectra, but instead I select random elements from the dataset as a whole.} and assume they are corrupted.

Applying the same procedure as above for the full dataset, I construct basis sets as a function of the number...
of components. Figure 3 presents the basis sets for \( n = 3 \) to \( n = 10 \). Remarkably, they are very similar to those basis sets learned from the full dataset. A careful comparison shows that there are some small differences on a few percent level, but it is reassuring that the algorithm can achieve such robust results.

To take a further look, I take the basis sets built from the partial dataset, and apply them to the full dataset to see how well they can describe the full dataset as a whole. The projection mode (with one factor fixed) of the algorithm makes this a trivial task. In the upper panel of Figure 4, I show the progression of the reduced \( \chi^2_{\text{red}} \) from this experiment. In the lower panel, I compare the cost to that with the basis sets learned from the full sample. The result shows that the basis sets built from the partial dataset, with 20% data masked, can account for the variance in the full dataset up to 98%.

Because the algorithm can handle missing data, it can be very useful in extragalactic astronomy. When we observe sources at different redshifts with a given instrument, the fixed observer-frame wavelength coverage translates to a running rest-frame window. If we use standard PCA or the original NMF, then we need to restrict the analysis to a small rest-frame wavelength range in which sources at different redshifts have common coverage. With the NMF technique described here, Zhu & Ménard (2013) modeled quasar spectra over a large redshift and rest-frame wavelength range (e.g., see their Figure 14), and I refer interested readers to that paper for more information about the application.

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4. SUMMARY

With the amount of data growing exponentially, one of the major challenges in modern astronomy is how to efficiently extract scientific information. I presented a simple vectorized algorithm for nonnegative matrix factorization (NMF) with nonuniform uncertainties and missing data, which can be easily implemented in any modern vector language. I released a Python implementation of the algorithm. Using an optical spectroscopic dataset of extragalactic sources as an example, I showed how the weighted cost progresses and converges as a function of the number of components, the only free parameter in the technique. I have also discussed how to take advantage of the independent, sequential update rules for the two factors.

As a final note, although techniques such as PCA and NMF are powerful tools that can reduce the dimensionality of the data and reveal intrinsic dimensions informative about the underlying correlations and physics, they still have some fundamental limitations. For example, the (linear) combinations of the basis components can occupy a part of the space that is otherwise empty in reality. As another example, these techniques attempt to find the basis components that dominate the variance (so as to minimize the least squares error), and a small number of extreme cases are often not included in the modeling. In astronomy, these cases are often the most interesting ones as they present the best opportunities for groundbreaking discoveries. These limitations could be catastrophic especially when we are facing low S/N data, which has become more and more common in the new era featuring large surveys. To overcome these limitations, we need to resort to other techniques, such as using a set of archetypes to represent all the instances in the dataset (e.g., Zhu 2016).
Nonnegative Matrix Factorization

ences (LAMOST), Los Alamos National Laboratory, the Max-Planck-Institute for Astronomy (MPIA), the Max-
Planck-Institute for Astrophysics (MPA), New Mexico
State University, Ohio State University, University of
Pittsburgh, University of Portsmouth, Princeton Uni-
versity, the United States Naval Observatory, and the
University of Washington.

APPENDIX

A. THE CODE

A.1. Install the package

I have implemented the algorithm for NMF described in Section 2.2.1 in Python 3, including options for sparse
matrices and projection mode. I share the code, with the name NonnegMFPy, on the repository hosting service GitHub.
Interested user can fork or clone the repository. For readers who are only interested in using the package, I have also
released the code on Python Package Index (PyPI) and one can install it with:

> pip install NonnegMFPy

We recommend installing it via pip unless the user is keen in helping further develop and maintain the package. The
repository webpage also includes documentation and a user guide of the package. The user can provide weight ($V$)
and mask ($M$) matrices to take into account the uncertainties and missing data. In addition, the code also includes
projection mode options, $H_{\text{only}}$ and $W_{\text{only}}$, to learn only $H$ or $W$, given $W$ or $H$.

A.2. Test the code

The test optical spectroscopic dataset I used in the paper is publicly available in fits format. Assuming we have
extracted the spectra matrix $\text{spec}$ and the inverse variance matrix $\text{ivar}$ from the dataset. The user can test the code
as follows.

> from NonnegMFPy import nmf
> g = nmf.NMF(spec, V=ivar, n_components=5)
> chi2, time_used = g.solveNMF()

If the user has already learned $W$ and wishes to learn $H$ only, one can simply set $H_{\text{only}} = True$:

> g = nmf.NMF(spec, V=ivar, W=W_known, n_components=5)
> chi2, time_used = g.solveNMF(H_only=True)

Note the dimensions need to be compatible.

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8 https://github.com/guangtunbenzhu/NonnegMFPy
9 See README on https://github.com/guangtunbenzhu/NonnegMFPy
10 http://fits.gsfc.nasa.gov/