Bi-level Optimization for hyperparameters in Nonnegative Matrix Factorizations

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Abstract

Hyperparameters (HPs) Optimization in machine learning algorithms represents an open problem with a direct impact on algorithm performances and on the knowledge extraction process from data. Matrix Decompositions (MDs) has recently gained more attention in data science as mathematical techniques able to capture latent information embedded in large datasets. MDs can be formalized as penalized optimization problems in which the tuning of the penalization HPs represents an issue. Current literature panorama does not provide any general framework addressing optimally conditions for the best configuration of HPs. In this work, we focus on the role the HPs play in the penalized Nonnegative Matrix Factorizations (NMF) context and on the importance of their correct selection. Using a bi-level optimization approach, HPs selection is considered from an optimization point of view and their choice is directly incorporated in the unsupervised algorithm as a part of the updating process. Either theorems of existence and convergence of numerical solutions, under appropriate assumptions, are studied and a novel algorithm, namely AltBi-Alternate bi-level Algorithm, is proposed to tune the penalization HP in NMF problems.

Keywords — Nonnegative matrix factorization; Hyperparameter Optimization; Penalization; Low-Rank approximation

MSC Classification — 65K10; 65F55; 68Q32; 68V20; 90C46; 46N10
1 Introduction

All learning models require that some hyperparameters (HPs), variables governing the learning approach, be set before starting the learning process from data. HPs tuning usually requires a lot of effort, it is a user-dependent process and affects the performance of the learning model itself [13]. Automated Hyperparameter Optimization (HPO) would bring a solution to these problems, providing more reproducible learning results and facilitating fairly comparisons between different learning models [2]. Practically, HPs selection is often based on trial-and-error approaches via Grid or Random Search methods, these are time consuming and typically guided by some performance metric (cross-validation on the training set or evaluation on a held-out validation set). Methods ranging from Black-Box to Bayesian or Gradient Based (GB) approaches have been recently developed. GB methods reduce the validation error computing or approximating the gradient w.r.t. HPs [4, 5, 38]. One of the ways to go through GB methods for HPO is to formalize the problem as a bi-level task [16, 41]. Bi-level programming solves an outer optimization problem subject to the optimality of an inner optimization one [1]. Formally, let $\mathcal{A}$ be a learning model with $p$ hyperparameters $\lambda \in \Lambda = \Lambda_1 \times \cdots \times \Lambda_p$, and $q$ parameters $w \in \Omega = \Omega_1 \times \cdots \times \Omega_q$ and let $X \in \mathbb{R}^{n \times m}$ with $n, m \in \mathbb{N}$ be an assigned data matrix; the bi-level HPO can be written as:

$$
\lambda^* = \arg \min_{\lambda \in \Lambda} \mathcal{F}(\mathcal{A}(w(\lambda), \lambda), X) \quad \text{s. t.} \quad w(\lambda) = \arg \min_w \mathcal{L}(\lambda, X), \tag{1.1}
$$

where $\mathcal{F}$ measures the goodness of the parameters $w$ obtained by the algorithm $\mathcal{A}$ set with HPs $\lambda$ on $X$ and $\mathcal{L}$ is an empirical loss. Usually the inner problem aims to the minimization of the empirical loss $\mathcal{L}$ while the outer problem is related to HPs. The implicit dependency of the outer problem on $\lambda$ makes (1.1) difficult to be solved. Recently, first order bi-level optimization techniques based on estimating the Jacobian $\frac{d\mathcal{F}(\lambda)}{d\lambda}$ via implicit or iterative differentiation have been proposed to solve (1.1) [16, 17, 38, 41]. In this paper, we combine these approaches to tackle the HPO related to Matrix Decomposition (MDs) in an unsupervised scenario. In particular, we focused our attention on Nonnegative Matrix Factorizations (NMF) and its sparseness constrained variants [8, 6, 12, 19, 23, 25, 34, 35, 39]. We regard these problems as penalized optimization tasks with penalization coefficients to be considered HPs, and we focus on their proper choice on HPO issue. Taking advantages from the bi-level HPO problem formulation we construct an alternate bi-level approach which includes the HP choice as part of the algorithm that computes the factors satisfying the NMF data approximation task under study. In the remainder of this section, preliminary concepts on NMF and sparsity constraints in it are shortly reviewed as well as the importance of the penalization HP for sparse NMF. Section 2 describes the novel bi-level formulation of the penalized NMF and its treatment via an alternate methodology based on the bi-level approach. Results on existence and convergence for this problem are considered and then used as bases to design a new algorithm, namely AltBi-Alternate Bi-level Algorithm in Section 3. It constitutes our proposal to numerically solve the HPO issue in NMF models with additional sparsity constraints. Section 4 illustrates the numerical results obtained using AltBi algorithm on different artificial and signal real datasets. Some conclusive remarks are sketched in Section 5.
1.1 Preliminaries

The name NMF is related to a group of methodologies aiming to approximate a nonnegative data matrix \( X \in \mathbb{R}^{n \times m} \) (with typically \( n > m \)) as the product of two nonnegative matrices, the basis matrix \( W \in \mathbb{R}^{n \times r} \) and the encoding (or coefficient) matrix \( H \in \mathbb{R}^{r \times m} \), so that \( X \approx WH \). The value \( r \) selecting the number of columns of \( W \) or rows for \( H \) is problem dependent and user-specified; it represents an example of HP connected with NMF. A general NMF problem can be formulated as an optimization task

\[
\min_{W \geq 0, H \geq 0} D_\beta(X, WH) = \min_{W \geq 0, H \geq 0} \sum_{i=1}^{n} \sum_{j=1}^{m} d_\beta(X_{ij}, (WH)_{ij}),
\]

where the objective function \( D_\beta(\cdot, \cdot) \) is a \( \beta \)-divergence assessing how good \( X \) is fitted by its reconstruction \( WH \). Either data properties and specific application domain influence the specific choice of \( D_\beta \) (popular divergences are the squared Frobenius norm for \( \beta = 2 \), the generalized Kullback-Leibler (KL) divergence for \( \beta = 1 \) and the Itakura-Saito divergence for \( \beta = 0 \)). In this paper we consider the KL divergence which corresponds to the maximum likelihood estimation under an independent Poisson assumption. NMF models (1.2) can be also enriched with additional constraints by introducing penalty terms

\[
\min_{W \geq 0, H \geq 0} D_\beta(X, WH) + \lambda_W \mathcal{R}_1(W) + \lambda_H \mathcal{R}_2(H),
\]

where \( \mathcal{R}_1 : \mathbb{R}^{n \times r} \rightarrow \mathbb{R} \) and \( \mathcal{R}_2 : \mathbb{R}^{r \times m} \rightarrow \mathbb{R} \) are some penalization functions enforcing specific properties on \( W \) and \( H \), respectively; \( \lambda_W \) and \( \lambda_H \) are some real penalization coefficients (i.e. HPs), balancing the bias-variance trade-off in approximating \( X \) and preserving additional constraints. It is assumed that HPs are not both null for the penalty to make sense and (1.3) allows to penalize either one or both variables, simultaneously. The problem of a proper selection of the penalization HPs is still an unsolved issue in constrained NMF.

We focus our attention on sparsity constraint enforced on the matrix factors. In fact, sparseness leads to several advantages; it allows some form of compression, improving the computational cost and the interpretative aspect when many features (the columns in \( X \)) are present and the model becomes very large. A large amount of zeros provides also a natural way to perform features extraction, prevent over-fitting and avoid modeling the intrinsic noise embedded in the data matrix \( X \). Nonnegativity of standard NMF factors naturally provides some sparse results, nevertheless because of the sparseness degree in each factor cannot be controlled, this property needs to be enforced with direct constraints \[20\].

Various penalty terms can be used to enforce sparsity in NMF. The \( \ell_0 \) “norm” constraints on \( W \) and \( H \) \[18\] is an example. It originates from the Lasso problem \[45\] and it has been extensively used to address computational issues in Machine Learning and Pattern Recognition. However, this penalization makes the associated objective function non-convex, non-smooth, discontinuous and globally non-differentiable, resulting in a NP-hard optimization problem \[1.3\]. Conversely, \( \ell_1 \) and \( \ell_2 \) norms are valid alternatives to \( \ell_0 \) thanks to their analytical properties\[49\]. Sparsity can also be imposed via the \( \ell_{1,2} \) norm used either as penalization

\[1\] \( \ell_1 \) norm is a convex, non smooth, global non differentiable function, whereas \( \ell_2 \) norm is a convex, smooth, global differentiable function
function [27] and objective functions [33, 40], and the so called Hoyer sparse NMF model, where the normalized ratio of $\ell_1$ and $\ell_2$ norm is adopted on the columns of $W$ and rows of $H$ [22]. In the following, the $\ell_1$ norm is used being quite efficient for discussing wide models.

1.2 The penalization HP in NMF

Tuning HPs in constrained NMF problem (1.3) is usually done using some static optimization mechanisms. Grid Search approaches solve several variants of the same problem associated to predefined discrete set of HP values and then choose the best one according to some empirical criteria. A well-known example can be found in literature in the context of gene expression analysis [24]. L-curve criterion and the Discrepancy Principle are also well-known empirical strategies for computing the value of the penalization in Tikhonov regularization [20, 21]. Other sophisticated strategies for tuning penalty HPs are based on of active-set approaches for Frobenius NMF problem with the Tikhonov regularization on $W$ [47]; Bayesian optimization solving the problem

$$\min_{H \geq 0, W \geq 0} D_\beta(X, WH) + R_1(L_W W) + R_2(H L_H),$$

(2.1)

where $R(H) = \text{Tr}(H^T EH) = \sum_i ||H_{i,:}||_2^2 = ||H||_{2,1}^2$, where $H_{i,:}$ is the $i$-th row of $H$, with $E \in \mathbb{R}^{r \times r}$ being the all-ones matrix that enforces sparsity on $H$'s columns was used in [48] using the squared norm $\ell_2$. This is an alternative approach to the norm $\ell_{1,2}$.

2 New Formulation

Even several approaches of varying complexity were proposed to tackle HPO in models (1.3), a uniform theory applicable to general objectives and penalty functions is still lacking. The results reported in this paper aim to fill this void.

The main contribution of this paper lies in the reformulation of model (1.3) as:

$$\min_{H \geq 0, W \geq 0} \frac{1}{2}||X - WH||_F^2 + \lambda \frac{1}{2} R(H),$$

(1.4)

where $R(H) = \text{Tr}(H^T EH) = \sum_i ||H_{i,:}||_1^2 = ||H||_{1,1}^2$, where $H_{i,:}$ is the $i$-th row of $H$, with $E \in \mathbb{R}^{r \times r}$ being the all-ones matrix that enforces sparsity on $H$'s columns was used in [48] using the squared norm $\ell_2$. This is an alternative approach to the norm $\ell_{1,2}$.
each variable separately. This makes alternate optimization techniques suitable to be incorporated into the minimization process to derive NMF updating each factors separately: firstly, \(W\) is fixed to estimate \(H\) and then \(H\) is fixed to estimate \(W\). To tune the penalization HP we choose to incorporate it simultaneously into the updating matrix factor process introducing a bi-level strategy on each row of \(W\).

To simplify the notation regarding each row of \(W\), we will use from now on the notations:

- \(w \in \mathbb{R}^r\) indicates the \(i\)-th row of \(W\);
- \(w(\lambda) \in \mathbb{R}^r\) the \(i\)-th row of \(W\) associated to \(\lambda\),
- \(w_k \in \mathbb{R}\) the \(k\)-th element of \(w\),
- \(\lambda \in \mathbb{R}^n\) the vector of diagonal elements of \(L\) and \(\lambda \in \mathbb{R}\) the \(i\)-th diagonal element of \(L\).

To solve problem (2.2), we firstly consider the simple minimization problem in \(H\) (for fixed \(W\)):

\[
\min_{H \geq 0} D_\beta(X, WH), \tag{2.3}
\]

followed by the bi-level task on \(w \in \mathbb{R}^r\), which reads for each row \(i = 1, \ldots, n\):

\[
\min \{ f(\lambda) : \lambda \in \Lambda \} \tag{2.4}
\]

\[
f(\lambda) = \inf \{ \mathcal{G}(w(\lambda), \lambda) : w(\lambda) \in \arg \min_{u \in \mathbb{R}^r} \mathcal{L}_\lambda(u) \}, \tag{2.5}
\]

where \(f\) is the so-called Response Function \(f : \lambda \mapsto \sum_{j=1}^m d_\beta(x_j, \sum_{a=1}^r w_a(\lambda)H_{aj})\) of the outer problem. The Error Function \(\mathcal{G}\) is the outer objective such that

\[
\mathcal{G} : \mathbb{R}^r \times \Lambda \rightarrow \mathbb{R} : (w, \lambda) \mapsto \sum_{j=1}^m d_\beta(X_j, \sum_{k=1}^r w_k(\lambda)H_{kj}), \tag{2.6}
\]

where \(X_j \in \mathbb{R}^m\) is the \(j\)-th row of \(X\), whereas for every \(\lambda \in \Lambda\), the Loss Function \(\mathcal{L}_\lambda\) is the inner objective

\[
\mathcal{L}_\lambda : \mathbb{R}^r \rightarrow \mathbb{R} : w \mapsto \sum_{j=1}^m d_\beta(X_j, \sum_{k=1}^r w_kH_{kj}) + \lambda \nu(w), \tag{2.7}
\]

where \(\nu : \mathbb{R}^r \rightarrow \mathbb{R}\) is the linear function such that \(\sum_{i=1}^n \lambda \nu(w) = R(LW)\). Figure 1 sketches the main ideas the HPO bi-level approach is based on. In the following section, we clarify how to handle each part of the optimization problems (2.3) and (2.4).

### 2.1 Finding the unpenalized factor

Different updates rules exist to solve (2.3) satisfying different requirements (fast convergence or easy implementation mechanisms); these range from Multiplicative to Additive Update rules \[3, 46\]. In this paper we focus on standard Multiplicative Updates (MU) proposed for NMF in \[29\], satisfying an easy implementation requirement and monotonic convergence. MU can be seen also as gradient-based method and it is based on scaling rules –in an iterative manner– initialization matrices by minimizing a so called auxiliary function, based on Expectation-Maximization and Richardson-Lucy algorithms \[10, 28, 37, 42, 43\]. To facilitate the minimization procedure, MU approaches use an
Figure 1: Outline of the proposed approach: $W$ is fixed to estimate $H$ totally and then $H$ is fixed to estimate $W$ and the Hypergradient $\nabla_\lambda f$ used to optimize $\lambda$ (Bi-level approach).

auxiliary function which is an easier formulation of $F$, it is an upper-approximation of the objective function and matches it in only one point.

Despite the slow convergence to local minima, the approach based on auxiliary function was frequently adopted to minimize different NMF problems, since it insured the nonnegativity of its factors (starting from nonnegative initial values) without any further handling [15, 29].

In the following, we review update rules and the corresponding theorems solving NMF problems for general $\beta$ divergence giving the particular results for cases based on the Frobenius norm, KL and Itakura-Saito divergences, which represent some of the most used objective functions in real applications. For all of these, details of the following theorem and related proofs can be found in [14, 15, 26, 29].

**Theorem 2.1.** For $0 \leq \beta \leq 2$, the general $\beta$-divergence is non-increasing under the following Multiplicative Update rules:

$$H \leftarrow H \star \frac{W^T((WH)^{[\beta-2]} \star X)}{W^T((WH)^{[\beta-1]}}$$

where $\star$ denotes the Hadamard product and ratio and exponential operations are element-wise.

In particular, the KL divergence is non-increasing for

$$H \leftarrow H \star \frac{W^T(X/(WH))}{(\sum_{i=1}^n W_{i,:})^T \star 1_m}$$

with $1_m$ the ones-vector of dimension $m$. 
Even if the update (2.8) has not been proven for $\beta < 0$ and $\beta > 2$, several experimental results empirically demonstrated it is still non-increasing so that an extension of results in Theorem 2.1 is still an open problem [15].

2.2 Finding the penalized factor and solving the HPO

To obtain the update for $W$ and determine an optimal solution for the penalization HP matrix $L$, we use the bi-level approach (2.4)-(2.5) applied on each row of $W$.

For the sake of simplicity, let us assume that the inner objective has a unique minimizer $w(\lambda)$ and the HPs are reals. Nevertheless problem (2.4)-(2.5) remains challenging to solve, as in general there is no closed expression for $w(\lambda)$, so it is not possible to directly optimize the outer objective function.

As mentioned before, depending on how the gradient is calculated with respect to HPs, there are two main types of approaches: the Implicit Differentiation that is based on the implicit function theorem, and the Iterative Differentiation approach that replaces the inner problem with a dynamical system. In this work, we will focus on this latter, reformulating it for the NMF problem (2.2).

In general, the solution of the inner objective minimization can be formulated as a dynamical system with a state $w(t) \in \mathbb{R}^r$ as:

$$w(t) = \Phi_t(w(t-1), \lambda) \quad t = 1, ..., T;$$

with the initial condition $w(0) = \Phi_0(\lambda)$, where for every $t = 1, \ldots, T$ the function $\Phi_t : (\mathbb{R}^r \times \mathbb{R}) \to \mathbb{R}^r$ is a smooth mapping. In our case, this function represents the update performed by the $t$-th step of the optimization algorithm, since $\Phi_t$ is a row-wise update for $W$. Observe that $w^{(1)}, \ldots, w^{(T)}$ implicitly depend on $\lambda$.

The bi-level problem (2.4)-(2.5) can be approximated (for each row $i = 1, \ldots, n$) by the following constrained procedure:

$$\min_{\lambda} f(\lambda) \quad \text{s. t.} \quad w^{(t)} = \Phi_t(w^{(t-1)}, \lambda) \quad \text{for} \quad t = 1, \ldots, T. \quad (2.11)$$

In general, the procedure (2.11), might not be the best approximation of the bi-level problems (2.4)-(2.5), because the optimization dynamics converge to some minimizer of the inner objective $E$, but not necessarily to the one that also minimizes the function $g$.

The situation is, however, different if the inner problem admits a unique minimizer for every $\lambda \in \Lambda \subset \mathbb{R}$. Indeed in this case, it is possible to show that the set of minimizers of the approximate problems converges, in an appropriate sense as $T \to +\infty$, to the set of minimizers of the bi-level problem. Moreover, we note also that for $1 \leq \beta \leq 2$, thanks to the convexity of the $\beta$ divergence function and, consequently, of $E$, the associated problems $\arg \min f^{(T)}(\lambda)$, $\arg \min f(\lambda)$ and $\arg \min E$ are singleton.

Now, results about the existence of solutions of problem (2.4)-(2.5) and the convergence for the approximate problem (2.11) related to them, can be provided under the following assumptions which allow us to rewrite the problem (2.11).

**Hypothesis 1.** The following assumptions will be used to prove the existence and convergence results:

1. $L_\lambda$ is convex as a sum of convex functions.

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1. the set Λ is a compact subset of \( \mathbb{R} \);

2. the Error Function \( E : \mathbb{R}^{r} \times \Lambda \to \mathbb{R} \) is jointly continuous;

3. the map \((w, \lambda) \to \mathcal{L}_{\lambda}(w)\) is jointly continuous and then the problem \(\arg\min \mathcal{L}_{\lambda}\) is a singleton for every \(\lambda \in \Lambda\);

4. the problem \(w(\lambda) = \arg\min \mathcal{L}_{\lambda}\) remains bounded as \(\lambda\) varies in \(\Lambda\).

Our problem formulation verifies the assumptions, according to which, the initial bi-level problem composed by (2.4)–(2.5) can be reformulated as in the following:

\[
\min_{\lambda \in \Lambda} f(\lambda) = E(w(\lambda^{*}), \lambda^{*}), \quad w(\lambda) = \arg\min_{u} \mathcal{L}_{\lambda}(u), \tag{2.12}
\]

where \((w(\lambda^{*}), \lambda^{*})\) is the optimal solution.

### 2.2.1 Existence and Convergence Results

In this section results about the existence of solutions of (2.12) and the (variational) convergence of the approximate problems (2.11) are proven.

**Theorem 2.2 (Existence).** The problem (2.12) admits solutions under the assumptions 1–4 in [7].

**Proof.** Since \(\Lambda\) is compact, from Weierstrass theorem, it follows that a sufficient condition for the existence of minimizers is that \(f\) is continuous. Consider \(\hat{\lambda} \in \Lambda\) and let \((\lambda_{n})_{n \in \mathbb{N}}\) be a sequence in \(\Lambda\) such that \(\lambda_{n} \to \hat{\lambda}\). Since the associated sequence \((w(\lambda_{n}))_{n \in \mathbb{N}}\) is bounded, there exists a subsequence \((w(\lambda_{kn}))_{n \in \mathbb{N}}\) such that \(w(\lambda_{kn}) \to \hat{w}\) for some \(\hat{w} \in \mathbb{R}^{r}\). Now, since \(\lambda_{kn} \to \hat{\lambda}\) and the map \((w, \lambda) \to \mathcal{L}_{\lambda}(w)\) is jointly continuous, we have

\[
\forall w \in \mathbb{R}^{r} \quad \mathcal{L}_{\hat{\lambda}}(\hat{w}) = \lim_{n} \mathcal{L}_{\lambda_{kn}}(w(\lambda_{kn})) \leq \lim_{n} \mathcal{L}_{\lambda_{kn}}(w) = \mathcal{L}_{\hat{\lambda}}(w). \tag{2.13}
\]

Thus, \(\hat{w}\) is a minimizer of \(\mathcal{L}_{\hat{\lambda}}\) and hence \(\hat{w} = w(\lambda)\) and this proves that \((w(\lambda_{n}))_{n \in \mathbb{N}}\) is a bounded sequence having a unique cluster point.

Hence \((w(\lambda_{n}))_{n \in \mathbb{N}}\) is convergent to its unique cluster point, which is \(w(\lambda)\).

Finally, since \((w(\lambda_{n}), \lambda_{n}) \to (w(\hat{\lambda}), \hat{\lambda})\) and the error function \(E\) is jointly continuous, it follows

\[
f(\lambda_{n}) = E(w(\lambda_{n}), \lambda_{n}) \to E(w(\hat{\lambda}), \hat{\lambda}) = f(\hat{\lambda}),
\]

that concludes the proof. \(\square\)

**Theorem 2.3 (Convergence).** In addition to hypothesis 1–4 in [7], suppose that:

5. \(E(\cdot, \lambda)\) is uniformly Lipschitz continuous;

6. The iterates \((w(T))_{T \in \mathbb{N}}\) converge uniformly to \(w(\lambda)\) on \(\Lambda\) as \(T \to +\infty\).

Then

(a) \(\inf f(T)(\lambda) \to \inf f(\lambda)\),

(b) \(\arg\min f(T)(\lambda) \to \arg\min f(\lambda)\), meaning that, for every \((\lambda_{T})_{T \in \mathbb{N}}\) such that \(\lambda_{T} \in \arg\min f(T)(\lambda)\), we have that:
\[(\lambda_T)^{T \in \mathbb{N}} \text{ admits a convergent subsequence;} \]

- for every subsequence \((\lambda_{K_T})^{T \in \mathbb{N}}\) such that \(\lambda_{K_T} \to \hat{\lambda}\), we have \(\hat{\lambda} \in \arg \min f(\lambda)\).

To prove Theorem 2.3, the following preliminary result concerning the stability of minima and minimizers in optimization problems are useful (the complete proof of this result can be found in [11]).

**Theorem 2.4.** Let \(g_{T}\) and \(g_{\lambda}\) be lower semicontinuous functions defined on a compact set \(\Lambda\). Suppose that \(g_{T}\) converges uniformly to \(g_{\lambda}\) on \(\Lambda\) as \(T \to +\infty\). Then

- \(\inf g_{T} \to \inf g\)
- \(\arg \min g_{T} \to \arg \min g\), meaning that, for every \((\lambda_{T})^{T \in \mathbb{N}}\) such that \(\lambda_{T} \in \arg \min g_{T}\), we have that:
  - \((\lambda_{T})^{T \in \mathbb{N}}\) admits a convergent subsequence;
  - for every subsequence \((\lambda_{K_{T}})^{T \in \mathbb{N}}\) such that \(\lambda_{K_{T}} \to \hat{\lambda}\), we have \(\hat{\lambda} \in \arg \min g_{\lambda}\).

Thanks to these results, Theorem 2.3 can be proved.

**Proof of Theorem 2.3.** Since \(E(\cdot, \lambda)\) is uniformly Lipschitz continuous, there exists \(\nu > 0\) such that for every \(T \in \mathbb{N}\) and every \(\lambda \in \Lambda\) results:

\[
|f(T)(\lambda) - f(\lambda)| = |E(w^{(T)}(\lambda), \lambda) - E(w(\lambda), \lambda)| \leq \nu ||w^{(T)}(\lambda) - w(\lambda)||.
\]

Then, from assumption \(f^{(T)}(\lambda)\) converges to \(f(\lambda)\) uniformly on \(\Lambda\) as \(T \to +\infty\). The statement follows from the previous Theorem 2.4.

It is worthy to underline that the hypotheses (1) – (6) are satisfied by many problems of practical interest, in particular in our case when \(1 \leq \beta \leq 2\). For the other \(\beta\) values we are studying these results even if we lose the hypothesis of convexity of \(f\) and \(L_{\lambda}\). However, we are confident that similar existence and convergence results can be found due to the fact that, for \(\beta < 1\) and \(\beta > 2\), \(f\) and \(L_{\lambda}\) can be rewritten by the sum of concave and convex functions.

### 2.2.2 Solving the bi-level Problem

The bi-level problem (2.4)-(2.5) verifies the existence and convergence theorems previously stated; hence now we can focus on practically finding the penalization HPs matrix \(L\). Supposing to apply a Gradient type approach on each diagonal element \(\lambda\) of \(L\), the optimization result, for \(\lambda \in \Lambda\), comes from the estimation of the gradient \(\nabla_{\lambda} f\), called Hypergradient. This is not directly dependent from \(\lambda\), hence by using the chain rule we obtain:

\[
\nabla_{\lambda} f = \frac{\partial f}{\partial \lambda} + \frac{\partial f}{\partial w^{(T)}} \cdot \frac{dw^{(T)}}{d\lambda},
\]

(2.14)

where \(\frac{\partial f}{\partial \lambda} \in \mathbb{R}\) and \(\frac{\partial f}{\partial w^{(T)}} \in \mathbb{R}^{r}\) are available. Considering \(w^{(T)}\) as a function of \(\lambda\), we can estimate Hypergradient by computing the row-vector product \(\frac{\partial f}{\partial w^{(T)}} \cdot \frac{dw^{(T)}}{d\lambda}\). Following an Iterative Differentiation approach, the computation of the Hypergradient can be done using reverse or forward mode. Reverse-Mode Differentiation (RMD) computes the Hypergradient by back-propagation, instead Forward-Mode Differentiation (FMD) works it by forward propagation. In our algorithm we use only the second mode, but, for completeness, we report both.
Reverse Mode  The reverse strategy to compute the Hypergradient is based on a Lagrangian perspective calculated for \(2.11\), that is \(\mathcal{L} : \mathbb{R}^r \times \Lambda \times \mathbb{R}^r \to \mathbb{R}\) which is defined as
\[
\mathcal{L}(w, \lambda, \alpha) = \mathcal{E}(w^{(T)}, \lambda) + \sum_{t=1}^{T} \alpha_t(\Phi_t(w^{(t-1)}, \lambda) - w^{(t)})
\]
where, for each \(t = 1, \ldots, T\), \(\alpha_t \in \mathbb{R}^r\) is a row vector of Lagrange multipliers associated with \(t\)-th step of the dynamics. The partial derivatives of the Lagrangian \(\mathcal{L}\) are
\[
\begin{align*}
\frac{\partial \mathcal{L}}{\partial \alpha_t} &= \Phi_t(w^{(t-1)}, \lambda) - w^{(t)}, \\
\frac{\partial \mathcal{L}}{\partial w} &= \alpha_t + A_t, \\
\frac{\partial \mathcal{L}}{\partial w^{(t)}} &= \nabla \mathcal{E}(w^{(T)}, \lambda) - \alpha_T,
\end{align*}
\]
where \(A_t = \frac{\partial \Phi_t(w^{(t-1)}, \lambda)}{\partial w^{(t-1)}} \in \mathbb{R}^{r \times r}\) and \(B_t = \frac{\partial \Phi_t(w^{(t-1)}, \lambda)}{\partial \lambda} \in \mathbb{R}^{r \times 1}\), for \(t = 1, \ldots, T\). Therefore, setting each derivative to zero, the optimality conditions give the iterative rules FMD:
\[
\begin{align*}
\alpha_T &= \nabla \mathcal{E}(w^{(T)}, \lambda), \\
h_T &= \frac{\partial f}{\partial \lambda}, \\
h_{t-1} &= h_t + B_t \alpha_t, \\
\alpha_{t-1} &= A_t \alpha_t,
\end{align*}
\]
for \(t = T, \ldots, 1\) and then the Hypergradient can be computed as \(\nabla_{\lambda} f = h_0\).

Forward-Mode  FMD uses the chain rule for the derivative of composite functions \(2.14\). The functions \(\Phi_t\) for \(t = 1, \ldots, T\) depend both on \(\lambda\), directly by its expression, and on the state \(w^{(t-1)}\) indirectly. Applying again the chain rule, for every \(t = 1, \ldots, T\), the derivative of the state with respect to \(\lambda\) is:
\[
dw^{(t)} = \frac{\partial \Phi_t(w^{(t-1)}, \lambda)}{\partial w^{(t-1)}} dw^{(t-1)} + \frac{\partial \Phi_t(w^{(t-1)}, \lambda)}{\partial \lambda}.
\]
Defining \(Z_t = \frac{dw^{(t)}}{\partial \lambda} \in \mathbb{R}^{r \times 1}\) for every \(t = 1, \ldots, T\), the iterative rules FMD are:
\[
\begin{align*}
Z_0 &= B_0; \\
Z_t &= A_t Z_{t-1} + B_t \quad t = 1, \ldots, T;
\end{align*}
\]
where \(A_t\) and \(B_t\) are defined as above, for every \(t = 1, \ldots, T\) and the Hypergradient for each row of \(W\) is
\[
\nabla_{\lambda} f = G_T \cdot Z_T \in \mathbb{R}, \quad \text{being} \quad G_T = \frac{\partial f}{\partial w^{(T)}} \in \mathbb{R}^r.
\]
By initializing \(Z_0 = 0\), the solution of \(2.18\) is actually the solution of the more general difference equation:
\[
\nabla_{\lambda} f(\lambda) = \frac{\partial f(\lambda)}{\partial w^{(T)}} (B_T + \sum_{t=0}^{T-1} \prod_{s=t+1}^{T} A_s) B_t).
\]
Computational considerations  Opting between RMD and FMD depends on balancing trade-off based on the size of \( w \) and \( \lambda \). RMD approach requires all \( \{w^{(t)}\}_{t=1,...,T} \) are stored in memory to compute \( A_t \) and \( B_t \) in the backward pass and therefore is suitable when the quantity \( r(T) \) is small. AltBi uses a FMD strategy, that requires time \( O(r(T)) \) and space \( O(r) \), for every row and for every iteration.

3  Alternate bi-level Algorithm-AltBi

In this section, the new algorithm Alternate bi-level Algorithm-AltBi presented for the particular case \( \beta = 1 \) and \( \ell_1 \) as penalty function in (2.2). It implements the procedures described in the previous sections, performing NMF bi-level problem which includes the automatic setting of the HP. As its name suggests, AltBi performs the optimization on \( H \) with (2.8) and on \( W \) alternately through the bi-level approach. To perform the bi-level approach on \( W \), it is necessary to consider sub-interval, called the bunch of arbitrary length \( T \). This bunch has been inspired by analytical considerations. In fact, it is known that a convergent sub-sequence can be extracted from any bounded sequence\(^4\) and even if this is clearly not unique, it is enough to consider any its sub-sequence to still have the same limit. The Algorithm 1 shows the pseudo-code for AltBi.

Algorithm 1: AltBi-Alternate Bi-level Algorithm

| Data: \( X \in \mathbb{R}^{n \times m} \), factorization rank \( r \). |
| Result: \( W^{(\text{MaxIter})} \in \mathbb{R}^{n \times r}_{++}, H^{(\text{MaxIter})} \in \mathbb{R}^{r \times m}_{++}, \lambda^* \). |
| Initial matrices \( W^{(0)} \in \mathbb{R}^{n \times r}_+, H^{(0)} \in \mathbb{R}^{m \times r}_+ \), \( L^{(0)} = \text{diag}(\lambda^{(0)}) \), \( T \) length of bunch.: |
| while \( (\text{err} > \text{tol}) \land (\text{iter} < \text{MaxIter}) \) do |
| \( H = \text{update}(X, W, H) \); |
| for \( t \) in \( T \) do |
| \( (w^{(t)}), \nabla f \) = bi-level update(\( X, \nabla \lambda^{(t-1)} f, w^{(t-1)} \), \( H \)) |
| end |
| \( \lambda^{\text{iter}} \) = update(\( \lambda^{\text{iter}-1}, \nabla \lambda^{\text{iter}-1} f \)); |
| \( \text{iter}+ = 1 \); |
| end |

It receives as input the data matrix \( X \), the rank of the factorization \( r \) and the initial matrices \( W^{(0)}, H^{(0)} \) and \( L^{(0)} \). This latter is given as a vector \( \lambda \) of the diagonal elements of \( L \). The number of iterates \( \text{MaxIter} \), the tolerance \( \text{tol} \) and the length \( T \) of the bunch are also initialized. The outer while-loop repeats the alternating algorithm until one of the two conditions \( \text{err} > \text{tol} \) or \( \text{iter} < \text{MaxIter} \) is false. Whereas the inner for-loop performs the bi-level procedure for every bunch, in which the Hypergradient is calculated to be used for updating \( \lambda \) with a gradient method. The algorithm returns the matrices \( W \) and \( H \) and the value of the optimal HP vector \( \lambda^{(\text{MaxIter})} = \lambda^* \).

Here we show the particular theoretical case, that is:

\[
\min_{H \geq 0, W \geq 0} D_1(X, WH) + ||LW||_1. \tag{3.1}
\]

\(^4\)This holds for the Bolzano-Weierstrass Theorem
As described before, we follow an alternate minimization approach. For the update rule we use the MU rule specified in (2.9). Instead, for the bi-level formulation we keep the KL divergence with the $\ell_1$ norm as Loss function in (2.7):

$$\mathcal{L}_\lambda : \mathbb{R}^r \to \mathbb{R} : w \mapsto \sum_{j=1}^{m} d_1(X_{ij}, \sum_{k=1}^{r} w_k H_{kj}) + \lambda \|w\|_1,$$

(3.2)

whereas the KL divergence is the error function of the outer problem (2.6):

$$\mathcal{E} : \mathbb{R}^r \times \Lambda \to \mathbb{R} : (w, \lambda) \mapsto \sum_{j=1}^{m} d_1(X_{ij}, \sum_{k=1}^{r} w_k(\lambda) H_{kj}),$$

(3.3)

To assess the theoretical results for the previous functions, hypothesis 1 needed to be verified. Observe that $\mathcal{E}$ is jointly continuous w.r.t. $w$ and $\lambda$. Similarly $d_3$ and the map $(w, \lambda) \mapsto \mathcal{L}$. From the convexity and the compactness of $\Lambda$, arg min $\mathcal{L}$ is a singleton for any $\lambda \in \Lambda$. Finally $w(\lambda) = \arg \min \mathcal{L}$ remains bounded as $\lambda$ varies in $\Lambda$, in fact:

$$\|w(\lambda)\| \leq M \quad \forall \lambda \in \Lambda \quad \text{with} \quad M > 0, \quad M \leq M^*,$$

being $M^* = \max\{\|w(\lambda)\|_2 \mid \lambda \in \Lambda\}$. The matrix $W$ is updated using the following novel rule by rows (this update can be derived similarly to results in [29, 30]).

$$\Phi_k(w^t) = w_k^{(t-1)} + \frac{\sum_{j=1}^{m} H_{kj} \ast (X_{ij}/\sum_{a=1}^{r} w_a H_{aj})}{\sum_{j=1}^{m} H_{kj} + \lambda}, \quad \text{for} \quad k = 1, \ldots, r.$$  

(3.4)

Its proof is detailed in Appendix A. The HP $\lambda$ is also updates by the steepest descent procedure:

$$\lambda^{s+1} = \lambda^s - t \nabla_{\lambda^{s-1}} D(\lambda^{s-1}), \quad s = 1, \ldots, S,$$

(3.5)

with $S$ the maximum number of iterations and $c_s = \frac{1}{s}$ the stepsize.

The Hypergradient $\nabla_{\lambda^{s-1}} D(\lambda^{s-1})$ in (2.19) can be expressed with

$$G_T(k) = -\sum_{j=1}^{m} \left( X_{ij} / \sum_{a=1}^{r} w_a^{(T)} H_{aj} \right) H_{kj} \quad \text{for} \quad k = 1, \ldots, r,$$

while $A_t^t$ and $B_t^t$ are given by:

$$A_{kh}^t = \begin{cases} \sum_{j=1}^{m} H_{kj}(X_{ij}/\sum_{a=1}^{r} w_a^{(t-1)} H_{aj}) - w_k^{(t-1)} \sum_{j=1}^{m} H_{kj}^2(X_{ij}/(\sum_{a=1}^{r} w_a^{(t-1)} H_{aj})^2) & \text{if} \ h = k \\ -w_k^{(t-1)} \sum_{j=1}^{m} H_{kj}(X_{ij}/(\sum_{a=1}^{r} w_a^{(t-1)} H_{aj})^2) H_{kj} & \text{if} \ h \neq k \end{cases}$$

$^5$The usual conditions on the stepsize are fulfilled

$$\sum_{s=1}^{S} c_s = \infty \quad \text{and} \quad \sum_{s=1}^{S} c_s^2 < \infty.$$
\[ B_k^t = -w_k^{(t-1)} \cdot \frac{\sum_{j=1}^m H_{kj} \cdot (X_{ij} / (\sum_{a=1}^r w_{a}^{(t-1)} H_{kj}))}{(\sum_{j=1}^m H_{kj} + \lambda)^2} \]

for \( t = 1, \ldots, T \).

Observe that, although we have focused on a specific objective function and its associated update rules, AltBi can be generalized to any \( \beta \)-divergence and penalization functions \( \mathcal{R} \) respecting the assumptions in Section 2.

4 Numerical Experiments

In this section, numerical results obtained using algorithm AltBi on two artificial and two real datasets are reported. AltBi algorithm has been implemented in MATLAB 2021a environment and numerical experiments were run on a 16Gb RAM, i7 octa core machine. Benchmarks used in the experiments are generated according to the model

\[ X \approx Y = WH. \quad (4.1) \]

A) Factor matrices were generated randomly as full rank uniform distributed matrices. Particularly, \( H \in \mathbb{R}_+^{r \times m} \) was generated using the MATLAB command \( \text{rand} \), while \( W \in \mathbb{R}_+^{n \times r} \) was generated using the MATLAB command \( \text{randn} \), to possess sparse columns. Negative entries were replaced with a zero-value. Finally a noiseless\(^6\) dataset \( Y \in \mathbb{R}_+^{n \times m} \) was constructed according to (4.1).

B) Each column in \( W \) is expressed as real sinusoidal wave signal with frequency and phase of set individually for each component/column. An example of this signal waveform is plotted in Figure 2a. The negative entries are replaced with a zero-value. The factor matrix \( H \) was randomly generated as full rank sparse matrix with the sparseness level \( \alpha_H \) adjusted by the user.

C) The source signals taken from the file AC10.art_spectr_noi of MATLAB toolbox NMFLAB for Signal Processing \(^7\) has been used. These signals form the matrix \( W \in \mathbb{R}_+^{n \times r} \). One signal waveform with \( n = 1000 \) and \( r = 5 \) is plotted in Figure 2b. Also in this case, \( H \) was generated as a sparse matrix with sparsity level fixed \( \alpha_H \).

D) Real reflectance signals taken from the U.S. Geological Survey (USGS) database\(^7\) has been used. The particular context of Hyperspectral unmixing aims to obtain basic components of the image, called endmembers and their corresponding proportions called abundances. Using the NMF model, the column vectors of \( W \) are feature vectors that contain the spectral signatures (endmembers) (Figure 2d) and \( H \) may represent the mixing matrix or vectorized abundance maps (Figure 2c). These signals are divided into 224 bands that cover the range of wavelengths from 400 \( nm \) to 2.5 \( \mu m \). The angle between any pair of the signals is greater than 15 degrees. These signals form the matrix \( W \in \mathbb{R}_+^{n \times r} \), where \( n = 224 \). The rank of factorization \( r \) determines the number of pure spectra.

\(^6\)Since our goal is to solve the identification problem, it is not necessary to perturb matrix \( Y \).

\(^7\)http://speclab.cr.usgs.gov/spectral.lib06
Figure 2: Waveform of signals in benchmark B (a), and benchmark C (b), Abundance maps (c) and Spectral signatures (d) of benchmark D.

Three NMF algorithms were used and compared: AltBi, the standard unpenalized MU in [31] and the standard penalized that alternates equations (2.9) and (1.2) (referred to P-MU) with \( \lambda = 0.5 \) fixed. All algorithms were initialized using the same random initializer generated from an uniform distribution. Efficiency of the methods is analysed performing 30 Monte Carlo (MC) runs of the NMF algorithms, each time the initial matrices \( W^{(0)} \) and \( H^{(0)} \) were different. The initial \( \lambda \) is chosen to have, at the beginning of the process, homogeneity between the terms characterizing the objective function, according to:

\[
\lambda^{(0)} = \frac{\sum_{j=1}^{m} d_1(X_{ij}; \sum_{k=1}^{r} w_k^{(0)} H_{kj}^{(0)})}{10 \cdot \rho(w^{(0)})}
\]

for \( i = 1, \ldots, n \); where \( \rho \) is the \( \ell_1 \) penalization norm in this particular experimental case. The maximum
number of iterations in all the algorithms was set to 1000 and the tolerance for early termination was equal to $10^{-6}$. The number of inner iterations (length of bunch) was set to 4, i.e., $T = 4$. The following tests were performed:

1) Benchmark A was used with $n = 1000$, $m = 50$, $r = 4$.
2) Benchmark B was used $n = 1000$, $m = 50$, $r = 4$, $\alpha_H = 0.1$.
3) Benchmark C was used with $n = 1000$, $m = 50$, $r = 5$, $\alpha_H = 0.1$.
4) Benchmark D was used with $n = 224$, $m = 3025$, $r = 5$.

In all tests no noisy perturbations were used.

Figure 3 reports the evolution of the Response and Objective functions w.r.t iterations for benchmark A. All other benchmarks present similar results as reported in Section 4.1.

![Figure 3: Evolution of Response (a) and Objective (b) functions w.r.t. iterations (Benchmarks A).](image)

The performance of the NMF algorithms was evaluated with the Signal-to-Interference Ratio (SIR) measure [dB] [9] between the estimated signals and the true ones. Figure 4 shows the SIR statistics for estimating the spectral signatures in the matrix $W$ and the abundance maps in matrix $H$ for the test A.

Table 1 reports the numerical results of Mean-SIR in estimating $W$ and $H$ for benchmark A.

The general structure of the optimized $\lambda$ has been also inspected. Figure 5 compares final and initial HP for benchmark A: pointwise and distribution of vector $\lambda$, Figures 5a and 5b, respectively. The peak for initial HP shifts, from nonzero to zero values. Therefore $\lambda$ is optimized as a sparse vector, so that the algorithm penalizes some rows of the $W$ rather than others.

Finally, numerical results are also compared evaluating the sparsity of $W$ and $H$ by
Figure 4: SIR statistics for estimating columns of $\mathbf{W}$ and rows $\mathbf{H}$ (Benchmark A).

Table 1: Mean-SIR [dB] for estimating the matrices $\mathbf{W}$ and $\mathbf{H}$.

| Algorithms     | SIR for $\mathbf{W}$ | SIR for $\mathbf{H}$ |
|----------------|-----------------------|-----------------------|
| MU            | 16.7325               | 19.2147               |
| P-MU          | 16.7325               | 19.2147               |
| AltBi         | 21.3388               | 23.3308               |

$\text{Sp}(\mathbf{A}) = 100 \cdot \frac{1 - \#(\mathbf{A} > \text{tol})}{\# \mathbf{A}}$, for $\mathbf{A} \in \mathbb{R}^{n \times m}$. Sparsity constraint was added only on $\mathbf{W}$ and for benchmarks C and D; the sparsity on $\mathbf{H}$ was provided by the user. As shown in Figure 6, the proposed method enforces the sparsity on $\mathbf{W}$ and does not affect the sparsity profile in $\mathbf{H}$, as is expected in our tests.

Observe that $\lambda^*$ obtained from AltBi provides the best results either in terms of identification and fitting problem. This fact, is even worthy, if one considers that the choice of $\lambda^*$ is automatic and no need to manually identify its best value is required. Figure 7 illustrates the behaviour the Response function for fixed values of $\lambda$ for the MU-P algorithm in comparison with the Non-penalized MU and AltBi. This latter shows the better performances.

4.1 Results for Benchmarks B, C, and D

All the experiments confirmed the expected behaviour of AltBi in term of an identification problem. In fact, Figures 8c, 9c and 10a show that the SIR values obtained with AltBi are significantly better than those obtained with MU and MU-P.

Moreover for benchmark D we show the original abundance maps (11a) and spectral signatures (11c) compared to the estimated abundance maps (11b) and spectral signatures (11d). Similar results are obtained for the Response and Objective functions in benchmark D, which we omit for the sake of brevity.

---

\[8\text{Sp}(\mathbf{A})\] represents the ratio between the complement of the number of elements greater than a certain tolerance and the total number of elements in matrix $\mathbf{A}$. 

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As we can observe, the abundance maps are estimated with lower SIR performance than the spectral signatures (matrix \( W \)) but this result is not surprising. This is because there is no penalty imposed on matrix \( H \). The sparsity-enforcing term was only considered for estimating matrix \( W \).

5 Conclusions

In this work a methodology based on two alternating phases is proposed for tuning penalization HPs in NMF tasks. It firstly solves the unpenalized factorization to obtain \( H \), then it alternates a second phase in which \( W \) and the penalization HPs matrix \( L \) are simultaneously get. Novelty of our HPO proposal is including the minimization of the penalization HP into the optimization problem in a bi-level fashion. Results on existence and convergence of solution to the considered tasks are also demonstrated; numerical experiments and comparisons are also promising.

HPO in an unsupervised scenario of data matrix factorization represents an evolving
Figure 7: Response Functions obtained through the MU-P algorithm with different λ values (0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1) compared with the unpenalized MU case and AltBi.

However, when the size of the problem is high, the computational cost required by AltBi could not make this algorithm competitive. To improve the computational efficiency a column-wise version of AltBi instead of row-wise is under study together with the possibility of speeding up the algorithm varying the length of the bunch variable to make local truncation error approximately constant.

Extension of theoretical results under hypotheses (1) – (6) when the convexity of error and loss function is lost are under consideration together with studies on the influence of different choices of the penalization functions and their effects on performances and computational for large dataset applications (such as Gene Expression analysis [12, 44], Blind Spectral Unmixing [32, 47] and Text Mining).

A Convergence and Correctness for the W update defined in (3.4)

Without loss of generality, function in (3.1) can be rewritten neglecting constants which are not relevant to the minimization process, that is:

$$
\sum_{i,j} \left( -X_{ij} \log (WH)_{ij} + (WH)_{ij} \right) + \lambda \sum_{ij} W_{ij}.
$$

(1.1)
In particular, we theorize its element-wise updates rules as:

\[ W_{ia} \leftarrow W_{ia} \frac{\sum_{j=1}^{m} (H_{aj} X_{ij}) / (WH)_{ij}}{\sum_{j=1}^{m} H_{aj} + \lambda}, \]  
\[(1.2)\]

for \( i = 1, \ldots, n \) and \( a = 1, \ldots, r \).

Being \( w \in \mathbb{R}^r \) and \( x \in \mathbb{R}^m \) the generic rows of \( W \) and \( X \), respectively, the function in (1.1) can be re-written with respect to the unknown \( w \) as

\[ F(w) = \sum_{j=1}^{m} -x_j \log \left( \sum_{a=1}^{r} w_a H_{aj} \right) + \sum_{j=1}^{m} \sum_{a=1}^{r} w_a H_{aj} + \lambda \sum_{a=1}^{r} w_a, \]
\[(1.3)\]

and then the updates for the unknown \( w \), in a row-wise formulation, follow from Theorem A.1.
Theorem A.1. The divergence in (1.3) is non-increasing under the update rules

$$w_a \leftarrow w_a \frac{\sum_{k=1}^{m} (H_{ak}x_k)/(\sum_{b=1}^{r} w_b H_{bk})}{\sum_{k=1}^{m} H_{ak} + \lambda},$$  \hspace{1cm} (1.4)$$

The divergence is invariant under these updates if and only if $\mathbf{w}$ is a stationary point of the divergence.

The following proof proceeds the demonstration scheme proposed by Lee and Seung [30] and Liu et al [36], but it adopts a different and more general formulation of the auxiliary function for the objective function (1.3).
Lemma A.2. $G(w, w^t) = \sum_{j=1}^m \sum_{a=1}^r w_a H_{aj}$

$$- \sum_{j=1}^m \sum_{a=1}^r x_j \frac{w^t_a H_{aj}}{\sum_{b=1}^r w^t_b H_{bj}} \left( \log (w_a H_{aj}) - \log \left( \frac{w^t_a H_{aj}}{\sum_{b=1}^r w^t_b H_{bj}} \right) \right) + \lambda \sum_{a=1}^r w_a$$

is an auxiliary function for $F(w)$.

Proof. We prove that $G(w, w^t)$ is an auxiliary function for $F(w)$. Due to the basic proprieties of logarithmic function, the condition $G(w, w) = F(w)$ is straightforward. To prove that $G(w, w^t) \geq F(w)$, we consider the quantity

$$\alpha_{aj} = \frac{w^t_a H_{aj}}{\sum_b w^t_b H_{bj}} \text{ with } \sum_j \sum_a \alpha_{aj} = 1. \quad (1.5)$$

Due to the convexity of the logarithmic function, the inequality

$$\sum_j x_j \log \frac{w_a H_{aj}}{\alpha_{aj}} - \sum_j \sum_a x_j \alpha_{aj} \log \left( \frac{w_a H_{aj}}{\alpha_{aj}} \right) \geq 0 \quad (1.6)$$

holds, so that the proof follows.

Lemma A.3. The objective function $F$ is non-increasing when its auxiliary function is minimized.

Proof. The minimum value of $G(w, w^t)$ with respect to $w$ satisfies

$$\frac{dG(w, w^t)}{dw_a} = \sum_j H_{aj} - \sum_j x_j \sum_b \frac{w^t_b H_{bj}}{H_{aj}} \left( \frac{1}{H_{aj}} \right) + \lambda = 0. \quad (1.7)$$
Thus, the update rule is

\[
    w_{i}^{t+1} \leftarrow w_{i}^{t} - \frac{\sum_{k=1}^{m} (H_{sk}x_k)/(\sum_{b=1}^{r} w_{i}^{b}H_{bk})}{\sum_{k=1}^{m} H_{sk} + \lambda},
\]

(1.8)

According to this new update, the KKT conditions w.r.t the nonnegative constraints, can be written as:

\[
    \begin{cases}
        W \ast \nabla_W F(W, H) = 0, \\
        \nabla_W F(W, H) \geq 0, \\
        W \geq 0,
    \end{cases}
\]

(1.9)
where \( \ast \) is the Hadamard point-wise product and \( \nabla_{\mathbf{w}} \) is the gradient of (1.1). This formulation allows to prove that the update (1.2) satisfies the KKT conditions (1.9) at the convergence, then its correctness is ensured.

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