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## Supporting Technical Report for the Article "Variational Bayesian Inference for Source Separation and Robust Feature Extraction"

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Kamil Adiloglu, Emmanuel Vincent. Supporting Technical Report for the Article "Variational Bayesian Inference for Source Separation and Robust Feature Extraction". [Technical Report] RT-0423, 2012, pp.25. hal-00687162v1

**HAL Id: hal-00687162**

**<https://inria.hal.science/hal-00687162v1>**

Submitted on 12 Apr 2012 (v1), last revised 25 Feb 2014 (v3)

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# Supporting Technical Report for the Article “Variational Bayesian Inference for Source Separation and Robust Feature Extraction”

Kamil Adilođlu, Emmanuel Vincent

**TECHNICAL  
REPORT**

**N° 423**

April 2012

Project-Team Metiss





## Supporting Technical Report for the Article “Variational Bayesian Inference for Source Separation and Robust Feature Extraction”

Kamil Adiloğlu, Emmanuel Vincent

Project-Team Metiss

Technical Report n° 423 — April 2012 — 22 pages

**Abstract:** This technical report presents the details of the derivation of the variational Bayesian source separation algorithm in [1]. For the motivation behind this algorithm and for experimental results, see [1].

**Key-words:** Audio source separation, local Gaussian modeling, non-negative matrix factorization, variational Bayesian inference

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This work is a part of the QUAERO project funded by OSEO.

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# Rapport Technique pour l'Article "Variational Bayesian Inference for Source Separation and Robust Feature Extraction"

**Résumé :** Ce rapport présente les détails de conception de l'algorithme variationnel bayésien pour la séparation de sources dans [1]. La motivation sous-jacente à cet algorithme et les résultats sont donnés dans [1].

**Mots-clés :** Séparation de sources audio, modèle gaussien local, factorisation matricielle positive, inférence variationnelle bayésienne

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# 1 Model

## 1.1 Spatial Model

We adopt the model proposed in [5]. This model operates in the STFT domain. The mixing equation in time frequency bin  $(n, f)$  can be formulated by using the source images  $\mathbf{y}_{j,fn}$  as follows:

$$\mathbf{x}_{fn} = \sum_{j=1}^J \mathbf{y}_{j,fn} + \boldsymbol{\epsilon}_{fn}. \quad (1)$$

In this domain,  $\mathbf{x}_{fn}$  represents the  $I \times 1$  vector containing the mixture STFT coefficients in time-frequency bin  $(n, f)$ , where  $I$  is the number of channels.  $\mathbf{y}_{j,fn}$  represents the  $I \times 1$  vector consisting of the spatial image of source  $j$  on all mixture channels in the same time-frequency bin. Finally  $\boldsymbol{\epsilon}_{fn}$  is the noise in the STFT domain. We assume that each source image follows a zero-mean complex-valued Gaussian distribution

$$\mathbf{y}_{j,fn} \sim \mathcal{N}(\mathbf{0}, v_{j,fn} \mathbf{R}_{j,f}), \quad (2)$$

where  $\mathbf{R}_{j,f}$  is an  $I \times I$  matrix of rank  $R_j$  which is called the spatial covariance matrix and represents the spatial characteristics of source  $j$  and of the mixing system, and  $v_{j,fn}$  is a scalar spectral power which represents the spectral characteristics of source  $j$ .

This model can alternatively be represented as follows [5].  $\mathbf{R}_{j,f}$  can be written as  $\mathbf{R}_{j,f} = \mathbf{A}_{j,f} \mathbf{A}_{j,f}^H$ , where  $\mathbf{A}_{j,f}$  is a  $I \times R_j$  dimensional complex-valued mixing matrix of rank  $R_j$  for source  $j$ . For each source  $j$ , we define  $R_j$  source components  $s_{jr,fn}$  distributed as

$$s_{jr,fn} \sim \mathcal{N}(0, v_{j,fn}). \quad (3)$$

Denoting by  $R = \sum_{j=1}^J R_j$  the total number of source components, the source coefficients can be formulated as

$$\mathbf{s}_{fn} = [s_{1,fn}^T, \dots, s_{j,fn}^T, \dots, s_{J,fn}^T]^T, \quad (4)$$

where  $\mathbf{s}_{fn}$  is an  $R \times 1$  vector of source coefficients with

$$\mathbf{s}_{j,fn} = [s_{j1,fn}, \dots, s_{jr,fn}, \dots, s_{jR_j,fn}]^T. \quad (5)$$

Hence, the prior distribution of the sources in time-frequency bin  $(f, n)$  is given by

$$\mathbf{s}_{fn} = \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_{s,fn}), \quad (6)$$

where  $\boldsymbol{\Sigma}_{s,fn}$  is an  $R \times R$  diagonal covariance matrix consisting of  $v_{j,fn}$  repeated  $R_j$  times for each source component  $s_{jr,fn}$  of source  $j$ . Finally, the mixing equation using the source components instead of the source spatial images as in (1) is given by

$$\mathbf{x}_{fn} = \mathbf{A}_f \mathbf{s}_{fn} + \boldsymbol{\epsilon}_{fn}. \quad (7)$$

We assume that the mixing system  $\mathbf{A}$  is stationary. So, the mixing system is expressed as

$$\mathbf{A}_f = [\mathbf{A}_{1,f}, \dots, \mathbf{A}_{j,f}, \dots, \mathbf{A}_{J,f}]. \quad (8)$$

Finally, we assume a Gaussian zero mean noise with a constant noise variance  $\epsilon_{fn} \sim \mathcal{N}(0, \Sigma_b)$ , where  $\Sigma_b = \sigma_b^2 \mathbf{I}$ . This gives us the possibility to formulate the likelihood of the mixture coefficients as follows:

$$p(\mathbf{X}|\mathbf{S}, \mathbf{A}) = \prod_{n=1}^N \prod_{f=1}^F \mathcal{N}(\mathbf{x}_{fn} | \mathbf{A}_f \mathbf{s}_{fn}, \sigma_b^2 \mathbf{I}), \quad (9)$$

where  $\mathbf{X} = \{\mathbf{x}_{fn}\}_{n=1 \dots N, f=1 \dots F}$  and  $\mathbf{S} = \{\mathbf{s}_{fn}\}_{n=1 \dots N, f=1 \dots F}$ .

## 1.2 Multilevel NMF as a Spectral Model

We assume a multilevel decomposition of the source variances  $v_{j,fn}$  in a non-negative matrix factorization (NMF) fashion [5]. In the first level we assume that the variances are the product of an excitation and a filter

$$v_{j,fn} = v_{j,fn}^{\text{ex}} v_{j,fn}^{\text{ft}}. \quad (10)$$

In the second and third levels,  $v_{j,fn}^{\text{ex}}$  is decomposed as follows:

$$v_{j,fn}^{\text{ex}} = \sum_{k=1}^{K_j^{\text{ex}}} \sum_{m=1}^{M_j^{\text{ex}}} \sum_{l=1}^{L_j^{\text{ex}}} h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} w_{j,fl}^{\text{ex}}, \quad (11)$$

where  $h_{j,mn}^{\text{ex}}$ ,  $g_{j,km}^{\text{ex}}$ ,  $u_{j,lk}^{\text{ex}}$  and  $w_{j,fl}^{\text{ex}}$  encode the temporal fine structure, the temporal envelope, the spectral envelope and the spectral fine structure respectively. The same decomposition is adapted for  $v_{j,fn}^{\text{ft}}$  as follows

$$v_{j,fn}^{\text{ft}} = \sum_{k'=1}^{K_j^{\text{ft}}} \sum_{m'=1}^{M_j^{\text{ft}}} \sum_{l'=1}^{L_j^{\text{ft}}} h_{j,m'n}^{\text{ft}} g_{j,k'm'}^{\text{ft}} u_{j,l'k'}^{\text{ft}} w_{j,fl'}^{\text{ft}}. \quad (12)$$

This multilevel NMF decomposition can be shown in matrix form as follows

$$\mathbf{V}_j = (\mathbf{W}_j^{\text{ex}} \mathbf{U}_j^{\text{ex}} \mathbf{G}_j^{\text{ex}} \mathbf{H}_j^{\text{ex}}) \odot (\mathbf{W}_j^{\text{ft}} \mathbf{U}_j^{\text{ft}} \mathbf{G}_j^{\text{ft}} \mathbf{H}_j^{\text{ft}}), \quad (13)$$

where  $\odot$  means element-wise matrix multiplication.

## 1.3 Prior Distributions for the Parameters

Each parameter may be fixed or adapted to the data. In a fully Bayesian treatment, we need to define the prior distributions for those parameters which are adapted to the data. We assume the NMF parameters of the source variances follow the non-informative Jeffreys prior  $\mathcal{J}(x) \propto \frac{1}{x}$



$$w_{j,fl}^{\text{ex}} \sim \mathcal{J}, \quad (14)$$

$$u_{j,lk}^{\text{ex}} \sim \mathcal{J}, \quad (15)$$

$$g_{j,km}^{\text{ex}} \sim \mathcal{J}, \quad (16)$$

$$h_{j,mn}^{\text{ex}} \sim \mathcal{J}, \quad (17)$$

$$w_{j,fl'}^{\text{ft}} \sim \mathcal{J}, \quad (18)$$

$$u_{j,l'k'}^{\text{ft}} \sim \mathcal{J}, \quad (19)$$

$$g_{j,k'm'}^{\text{ft}} \sim \mathcal{J}, \quad (20)$$

$$h_{j,m'n}^{\text{ft}} \sim \mathcal{J}. \quad (21)$$

For the mixing system, we take the dependencies between the channels and between the source components into account. Therefore, we consider the mixing matrix  $\mathbf{A}_f$  as a whole and define the prior distribution accordingly. First, we reshape the mixing matrix  $\mathbf{A}_f$  into a vector  $\underline{\mathbf{A}}_f$ . For this, we concatenate the row vectors of  $\mathbf{A}_f$  into the column vector  $\underline{\mathbf{A}}_f$ . Then, we define the prior distribution of  $\underline{\mathbf{A}}_f$  to be a complex multivariate Gaussian distribution as follows

$$\underline{\mathbf{A}}_f \sim \mathcal{N}(\mu_{\underline{\mathbf{A}},f}, \Sigma_{\underline{\mathbf{A}},f}). \quad (22)$$

In the following, we assume that  $\Sigma_{\underline{\mathbf{A}},f} \rightarrow +\infty$  so that this prior is actually flat.

## 1.4 Joint Distribution

With this prior information assumed, we can formulate the joint distribution  $p(\mathbf{X}, \mathbf{Z})$ , where  $\mathbf{Z}$  is the set of all model parameters

$$\mathbf{Z} = \{\mathbf{S}, \mathbf{A}, \mathbf{W}^{\text{ex}}, \mathbf{U}^{\text{ex}}, \mathbf{G}^{\text{ex}}, \mathbf{H}^{\text{ex}}, \mathbf{W}^{\text{ft}}, \mathbf{U}^{\text{ft}}, \mathbf{G}^{\text{ft}}, \mathbf{H}^{\text{ft}}\}. \quad (23)$$

as

$$\begin{aligned} p(\mathbf{X}, \mathbf{Z}) &= p(\mathbf{X}|\mathbf{S}, \mathbf{A})p(\mathbf{S}|\mathbf{W}^{\text{ex}}, \mathbf{U}^{\text{ex}}, \mathbf{G}^{\text{ex}}, \mathbf{H}^{\text{ex}}, \mathbf{W}^{\text{ft}}, \mathbf{U}^{\text{ft}}, \mathbf{G}^{\text{ft}}, \mathbf{H}^{\text{ft}})p(\mathbf{A}) \\ &\quad p(\mathbf{W}^{\text{ex}})p(\mathbf{U}^{\text{ex}})p(\mathbf{G}^{\text{ex}})p(\mathbf{H}^{\text{ex}})p(\mathbf{W}^{\text{ft}})p(\mathbf{U}^{\text{ft}})p(\mathbf{G}^{\text{ft}})p(\mathbf{H}^{\text{ft}}). \end{aligned} \quad (24)$$

The log-distribution is then given by

$$\begin{aligned}
\log p(\mathbf{X}, \mathbf{Z}) &= \log p(\mathbf{X}|\mathbf{S}, \mathbf{A}) + \log p(\mathbf{S}|\mathbf{W}^{\text{ex}}, \mathbf{U}^{\text{ex}}, \mathbf{G}^{\text{ex}}, \mathbf{H}^{\text{ex}}, \mathbf{W}^{\text{ft}}, \mathbf{U}^{\text{ft}}, \mathbf{G}^{\text{ft}}, \mathbf{H}^{\text{ft}}) \\
&\quad + \log p(\mathbf{A}) + \log p(\mathbf{W}^{\text{ex}}) + \log p(\mathbf{U}^{\text{ex}}) + \log p(\mathbf{G}^{\text{ex}}) + \log p(\mathbf{H}^{\text{ex}}) \\
&\quad + \log p(\mathbf{W}^{\text{ft}}) + \log p(\mathbf{U}^{\text{ft}}) + \log p(\mathbf{G}^{\text{ft}}) + \log p(\mathbf{H}^{\text{ft}}), \\
&= \sum_{f,n} \log \mathcal{N}(\mathbf{x}_{fn} | \mathbf{A}_f \mathbf{s}_{fn}, \sigma_b^2 \mathbf{I}) \\
&\quad + \sum_{f,n} \log \mathcal{N}(\mathbf{s}_{fn} | 0, \boldsymbol{\Sigma}_{s,fn}) \\
&\quad + \sum_{j,f,l} \log \mathcal{J}(w_{j,fl}^{\text{ex}}) \\
&\quad + \sum_{j,l,k} \log \mathcal{J}(u_{j,lk}^{\text{ex}}) \\
&\quad + \sum_{j,k,m} \log \mathcal{J}(g_{j,km}^{\text{ex}}) \\
&\quad + \sum_{j,m,n} \log \mathcal{J}(h_{j,mn}^{\text{ex}}) \\
&\quad + \sum_{j,f,l'} \log \mathcal{J}(w_{j,fl'}^{\text{ft}}) \\
&\quad + \sum_{j,l',k'} \log \mathcal{J}(u_{j,l'k'}^{\text{ft}}) \\
&\quad + \sum_{j,k',m'} \log \mathcal{J}(g_{j,k'm'}^{\text{ft}}) \\
&\quad + \sum_{j,m',n} \log \mathcal{J}(h_{j,m'n}^{\text{ft}}) \\
&\quad + \sum_f \log \mathcal{N}(\underline{\mathbf{A}}_f | \mu_{\underline{\mathbf{A}},f}, \boldsymbol{\Sigma}_{\underline{\mathbf{A}},f}). \tag{25}
\end{aligned}$$

## 2 Variational Inference

We aim to obtain the posterior distribution of the model parameters  $p(\mathbf{Z}|\mathbf{X})$ . However exact Bayesian inference is intractable. Therefore we resort to a variational Bayesian approximation [2].

### 2.1 General Approach

Marginalizing out the model parameters  $\mathbf{Z}$  from (24) gives us the marginal likelihood  $p(\mathbf{X})$  or the so-called evidence. We can also formulate the log marginal likelihood as follows:

$$\log p(\mathbf{X}) = \mathcal{L}(q) + KL(q||p), \quad (26)$$

where

$$\mathcal{L}(q) = \int q(\mathbf{Z}) \log \frac{p(\mathbf{X}, \mathbf{Z})}{q(\mathbf{Z})} d\mathbf{Z}, \quad (27)$$

$$KL(q||p) = - \int q(\mathbf{Z}) \log \frac{p(\mathbf{Z}|\mathbf{X})}{q(\mathbf{Z})} d\mathbf{Z}. \quad (28)$$

In this formulation,  $q(\mathbf{Z})$  is the joint distribution of the model parameters which we use to approximate the true posterior distribution  $p(\mathbf{Z}|\mathbf{X})$ .  $\mathcal{L}(q)$  is called the free energy and it is a lower bound of the marginal likelihood. Maximizing this free energy wrt.  $q(\mathbf{Z})$  minimizes the KL-divergence between the approximating distribution  $q(\mathbf{Z})$  and the true posterior [2]. Note that the KL-divergence vanishes when  $q(\mathbf{Z})$  is equal to the true posterior.

From now on, we assume the following factorization of the variational distribution  $q(\mathbf{Z})$ :

$$q(\mathbf{Z}) = \prod_{i=1}^M q_i(\mathbf{Z}_i). \quad (29)$$

If we embed this factorization into the free energy given in (27) and dissect out the dependency on one of the factors  $q_i(\mathbf{Z}_i)$ , we obtain

$$\mathcal{L}(q) = \int q_i \left\{ \int \log p(\mathbf{X}, \mathbf{Z}) \prod_{i' \neq i} q_{i'} d\mathbf{Z}_{i'} \right\} d\mathbf{Z}_i - \int q_i \log q_i d\mathbf{Z}_i + \text{const}, \quad (30)$$

$$= \int q_i \log \tilde{p}(\mathbf{X}, \mathbf{Z}_i) d\mathbf{Z}_i - \int q_i \log q_i d\mathbf{Z}_i + \text{const}, \quad (31)$$

$$= \int q_i \log \frac{\tilde{p}(\mathbf{X}, \mathbf{Z}_i)}{q_i} d\mathbf{Z}_i + \text{const}, \quad (32)$$

where

$$\log \tilde{p}(\mathbf{X}, \mathbf{Z}_i) = \int \log p(\mathbf{X}, \mathbf{Z}) \prod_{i' \neq i} q_{i'} d\mathbf{Z}_{i'} + \text{const}, \quad (33)$$

$$= \mathbb{E}_{i' \neq i} [\log p(\mathbf{X}, \mathbf{Z})] + \text{const} \quad (34)$$

and the normalizing constant is such that  $\tilde{p}(\mathbf{X}, \mathbf{Z}_i)$  is a proper distribution.

Now, suppose that we keep  $q_{i' \neq i}$  constant and maximize the free energy shown in (27) wrt.  $q_i$ . The minimum occurs when  $q_i(\mathbf{Z}_i) = \tilde{p}(\mathbf{X}, \mathbf{Z}_i)$ . As a result, we obtain a general equation for the solution maximizing the free energy as follows

$$q_i^*(\mathbf{Z}_i) = \tilde{p}(\mathbf{X}, \mathbf{Z}_i). \quad (35)$$

Note that in this equation, the update equation of the optimal approximating distribution  $q_i^*(\mathbf{Z}_i)$  depends on the expectation of the log of the joint distribution wrt. all other variational distributions. In that sense, (35) indicates a set of equations for  $i = \{1, \dots, M\}$ . Therefore an iterative update procedure is needed. After proper initialization of all the variational distributions, each distribution is updated in an iterative cycle.

In practice, (35) is applicable only when  $\mathbb{E}_{i' \neq i}[\log p(\mathbf{X}, \mathbf{Z})]$  is computable in closed form and corresponds to a known parametric distribution for which the normalizing constant is computable in closed form. When this is not the case,  $p(\mathbf{X}, \mathbf{Z})$  must be replaced by a lower bound for which the resulting approximating distribution becomes tractable.

Let us consider a parametric the lower bound  $f(\mathbf{X}, \mathbf{Z}, \Omega)$  of  $p(\mathbf{X}, \mathbf{Z})$  such that

$$p(\mathbf{X}, \mathbf{Z}) \geq f(\mathbf{X}, \mathbf{Z}, \Omega), \quad (36)$$

where  $\Omega$  is a set of auxiliary variables. Using this definition, we define  $\mathcal{B}$ , which further lower bounds  $\mathcal{L}$  as in the following

$$\mathcal{L}(q) \geq \mathcal{B}(q, \Omega) = \int q(\mathbf{Z}) \log \frac{f(\mathbf{X}, \mathbf{Z}, \Omega)}{q(\mathbf{Z})} d\mathbf{Z}. \quad (37)$$

Using  $\mathcal{B}(q, \Omega)$ , we rewrite the marginal distribution given in (26) as follows

$$\log p(\mathbf{X}) = \max_{\Omega} \mathcal{B}(q, \Omega) + (\mathcal{L}(q) - \max_{\Omega} \mathcal{B}(q, \Omega)) + KL(q||p). \quad (38)$$

Here we maximize the lower bound  $\mathcal{B}(q, \Omega)$  wrt.  $\Omega$ , which tightens the lower bound to the free energy  $\mathcal{L}(q)$ . Using the factorization we introduced in (29) and dissecting out the dependency on one of the factors  $q_i(\mathbf{Z}_i)$ , we obtain

$$\mathcal{B}(q, \Omega) = \int q_i \log \frac{\tilde{f}(\mathbf{X}, \mathbf{Z}_i, \Omega)}{q_i} d\mathbf{Z}_i + \text{const}, \quad (39)$$

where  $\log \tilde{f}(\mathbf{X}, \mathbf{Z}_i, \Omega)$  is defined as

$$\begin{aligned} \log \tilde{f}(\mathbf{X}, \mathbf{Z}_i, \Omega) &= \int \log f(\mathbf{X}, \mathbf{Z}, \Omega) \prod_{i' \neq i} q_{i'} d\mathbf{Z}_{i'} + \text{const}, \\ &= \mathbb{E}_{i' \neq i}[\log f(\mathbf{X}, \mathbf{Z}, \Omega)] + \text{const}, \end{aligned} \quad (40)$$

where the normalizing constant is such that  $\tilde{f}(\mathbf{X}, \mathbf{Z}_i, \Omega)$  is a proper probability distribution.

Hence, maximizing the lower bound  $\mathcal{B}(q, \Omega)$  wrt.  $q_i(\mathbf{Z}_i)$  minimizes an approximation to the KL-divergence between  $q(\mathbf{Z})$  and the true posterior distribution  $p(\mathbf{Z}|\mathbf{X})$ .

Finally, we conclude that two alternative steps yields the general equation for the optimal approximating distributions  $q_i^*$ . In the first step, we maximize the lower bound  $\mathcal{B}(q, \mathbf{\Omega})$  to the free energy  $\mathcal{L}(q)$  wrt. the auxiliary variables  $\mathbf{\Omega}$ , which tightens the lower bound, and in the second step, we maximize  $\mathcal{B}(q, \mathbf{\Omega})$  wrt. the approximating distributions  $q_i$ .

The optimal approximating distribution  $q_i^*(\mathbf{Z}_i)$  is given by

$$q_i^*(\mathbf{Z}_i) = \tilde{f}(\mathbf{X}, \mathbf{Z}_i, \mathbf{\Omega}). \quad (41)$$

In the following, we adopt this strategy for the derivation of the approximating distributions of the multilevel NMF parameters and the source components since  $\mathbb{E}[\log p(\mathbf{S}|\mathbf{V})]$  is not tractable in closed form as we will show in Section 2.2.1.

## 2.2 Application to the Considered Model

Pursuing this approach, we can factorize our  $q(\mathbf{Z})$  as follows:

$$\begin{aligned} q(\mathbf{Z}) = & \left( \prod_{f,n} q(\mathbf{s}_{fn}) \right) \\ & \left( \prod_f q(\mathbf{A}_f) \right) \\ & \left( \prod_{j,m,n} q(h_{j,mn}^{\text{ex}}) \right) \\ & \left( \prod_{j,k,m} q(g_{j,km}^{\text{ex}}) \right) \\ & \left( \prod_{j,k,l} q(u_{j,lk}^{\text{ex}}) \right) \\ & \left( \prod_{j,f,l} q(w_{j,fl}^{\text{ex}}) \right) \\ & \left( \prod_{j,m',n} q(h_{j,m'n}^{\text{ft}}) \right) \\ & \left( \prod_{j,k',m'} q(g_{j,k'm'}^{\text{ft}}) \right) \\ & \left( \prod_{j,k',l'} q(u_{j,l'k'}^{\text{ft}}) \right) \\ & \left( \prod_{j,f,l'} q(w_{j,fl'}^{\text{ft}}) \right). \end{aligned} \quad (42)$$

### 2.2.1 Auxiliary Variables

Let us define  $\eta = \{k, m, l\}$  the joint index of the excitation multilevel NMF parameters and  $\eta' = \{k', m', l'\}$  the joint index of the filter multilevel NMF parameters. With these joint indices let us further define  $v_{j,fn,\eta,\eta'}$  as the product

of the multilevel NMF parameters

$$v_{j,fn,\eta,\eta'} = h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} w_{j,fl}^{\text{ex}} h_{j,m'n}^{\text{ft}} g_{j,k'm'}^{\text{ft}} u_{j,l'k'}^{\text{ft}} w_{j,fl'}^{\text{ft}}. \quad (43)$$

Let us further define  $v_{j,fn,\eta}^{\text{ex}}$  as the product of the excitation coefficients of the multilevel NMF components and  $v_{j,fn,\eta'}^{\text{ft}}$  as the product of the filter coefficients

$$v_{j,fn,\eta}^{\text{ex}} = h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} w_{j,fl}^{\text{ex}}, \quad (44)$$

$$v_{j,fn,\eta'}^{\text{ft}} = h_{j,m'n}^{\text{ft}} g_{j,k'm'}^{\text{ft}} u_{j,l'k'}^{\text{ft}} w_{j,fl'}^{\text{ft}}. \quad (45)$$

Having these variables defined for the sake of readability, let us have a look at  $\mathbb{E}[\log p(\mathbf{S}|\mathbf{V})]$  more closely.

$$\begin{aligned} \mathbb{E}[\log p(\mathbf{S}|\mathbf{V})] &= \mathbb{E}\left[\log \prod_{f,n} \mathcal{N}(\mathbf{s}_{fn}|0, \Sigma_{\mathbf{s},fn})\right] \\ &= \mathbb{E}\left[\sum_{f,n} \log \mathcal{N}(\mathbf{s}_{fn}|0, \text{diag}(\sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'}))\right], \\ &= \mathbb{E}\left[\sum_{f,n} -R \log \pi - \log \det(\text{diag}(\sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'}))\right. \\ &\quad \left. - \mathbf{s}_{fn}^H \text{diag}(\sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'})^{-1} \mathbf{s}_{fn}\right], \\ &= \sum_{f,n} -R \log \pi + \sum_j -R_j \mathbb{E}\left[\log \sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'}\right] \\ &\quad + \sum_{j,r} -\mathbb{E}[|s_{jr,fn}|^2] \mathbb{E}\left[\frac{1}{\sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'}}\right]. \end{aligned} \quad (46)$$

As one can easily see, none of the two expectations in this equation above is tractable. So, we resort to the alternative method, which we introduced in Section 2.1 and lower bound  $p(\mathbf{S}|\mathbf{V})$  as explained in the following [3]. For the first expectation, we know that  $x \rightarrow -\log x$  is convex. So, we can lower bound it by its first-order Taylor series expansion around an arbitrary positive point  $\omega_{j,fn}$  as follows

$$\begin{aligned} -\log \sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'} &\geq -\log \omega_{j,fn} - \frac{1}{\omega_{j,fn}} (\sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'} - \omega_{j,fn}), \\ &= -\log \omega_{j,fn} + 1 - \frac{1}{\omega_{j,fn}} \sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'}. \end{aligned} \quad (47)$$

For the second expectation, we know that  $x \rightarrow \frac{-1}{x}$  is concave. So, for any positive  $\phi_{j,fn,\eta,\eta'}$  such that  $\sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'} = 1$ , using Jensen's inequality:

$$\begin{aligned} -\frac{1}{\sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'}} &= -\frac{1}{\sum_k \phi_{j,fn,\eta,\eta'} \frac{v_{j,fn,\eta,\eta'}}{\phi_{j,fn,\eta,\eta'}}} \\ &\geq -\sum_k \phi_{j,fn,\eta,\eta'} \frac{1}{\frac{v_{j,fn,\eta,\eta'}}{\phi_{j,fn,\eta,\eta'}}} \\ &= -\sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'}^2 \frac{1}{v_{j,fn,\eta,\eta'}}. \end{aligned} \quad (48)$$

Using these two inequalities, we can lower bound  $\log p(\mathbf{S}|\mathbf{V})$  using the auxiliary variables  $\boldsymbol{\Omega} = \{\{\omega_{j,fn}\}_{j,fn}, \{\phi_{j,fn,\eta,\eta'}\}_{j,fn,\eta,\eta'}\}$  as follows

$$\begin{aligned} \log p(\mathbf{S}|\mathbf{V}) &\geq -F \cdot N \cdot R \cdot \log \pi \\ &+ \sum_{j,fn} R_j \left( -\log \omega_{j,fn} + 1 - \frac{1}{\omega_{j,fn}} \sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'} \right) \\ &+ \sum_{j,fn} \sum_r -|s_{jr,fn}|^2 \sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'}^2 \frac{1}{v_{j,fn,\eta,\eta'}}. \end{aligned} \quad (49)$$

### 2.2.2 Tightening the Bound wrt. the Auxiliary Variables

Concerning  $\omega_{j,fn}$ , we simply take the partial derivative of the bound  $\mathcal{B}$  wrt.  $\omega$  which is given by

$$\begin{aligned} \mathcal{B} &= -F \cdot N \cdot R \cdot \log \pi \\ &+ \sum_{j,fn} R_j \left( -\log \omega_{j,fn} + 1 - \frac{1}{\omega_{j,fn}} \sum_{\eta} \sum_{\eta'} \mathbb{E}[v_{j,fn,\eta,\eta'}] \right) \\ &+ \sum_{j,fn} \sum_r -|s_{jr,fn}|^2 \sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'}^2 \mathbb{E} \left[ \frac{1}{v_{j,fn,\eta,\eta'}} \right] + \text{const.} \end{aligned} \quad (50)$$

So, the derivative is given as

$$\frac{\partial \mathcal{B}}{\partial \omega_{j,fn}} = -\frac{R_j}{\omega_{j,fn}} + \frac{R_j}{\omega_{j,fn}^2} \sum_{\eta} \sum_{\eta'} \mathbb{E}[v_{j,fn,\eta,\eta'}] \quad (51)$$

and make it equal to zero, which yields

$$\omega_{j,fn} = \sum_{\eta} \sum_{\eta'} \mathbb{E}[v_{j,fn,\eta,\eta'}]. \quad (52)$$

For  $\phi_{j,fn,\eta,\eta'}$ , we use Lagrange multipliers  $\delta_{j,fn}$ , because of the constraint. The Lagrangian is given by

$$\begin{aligned} \mathcal{B} &= \sum_{j,fn} \left( \sum_r -\mathbb{E}[|s_{jr,fn}|^2] \right) \sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'}^2 \mathbb{E} \left[ \frac{1}{v_{j,fn,\eta,\eta'}} \right] \\ &+ \delta_{j,fn} \left( \left( \sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'} \right) - 1 \right) + \text{const.} \end{aligned} \quad (53)$$

Taking the partial derivative with respect to  $\phi_{j,fn,\eta,\eta'}$  and  $\delta_{j,fn}$  yields the following system of equations:

$$\frac{\partial \mathcal{B}}{\partial \phi_{j,fn,\eta,\eta'}} = \left( \sum_r -\mathbb{E}[|s_{jr,fn}|^2] \right) \left( \sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'}^2 \mathbb{E} \left[ \frac{1}{v_{j,fn,\eta,\eta'}} \right] \right) \quad (54)$$

$$\frac{\partial \mathcal{B}}{\partial \delta_{j,fn}} = \left( \sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'} \right) - 1. \quad (55)$$

Solving the system for  $\phi_{j,fn,\eta,\eta'}$  yields

$$\phi_{j,fn,\eta,\eta'} = \frac{1}{C_{j,fn}} \mathbb{E} \left[ \frac{1}{v_{j,fn,\eta,\eta'}} \right]^{-1}, \quad (56)$$

where  $C_{j,fn}$  is the normalization constant given by

$$C_{j,fn} = \sum_{\eta} \sum_{\eta'} \mathbb{E} \left[ \frac{1}{v_{j,fn,\eta,\eta'}} \right]^{-1}. \quad (57)$$

### 2.2.3 Variational Updates for the Multilevel NMF Parameters

In this section, we will determine the approximating  $q$  distributions of the multilevel NMF parameters and derive the corresponding update equations. For this we will use the template given in (40, 41).

**Update Equations for  $w_{j,fl}^{\text{ex}}$ :** The probability distribution  $\tilde{f}(\mathbf{X}, w_{j,fl}^{\text{ex}}, \mathbf{\Omega})$  defined in (40) is given by

$$\begin{aligned} \log \tilde{f}(\mathbf{X}, w_{j,fl}^{\text{ex}}, \mathbf{\Omega}) &= \sum_n R_j \left( -\log \omega_{j,fn} + 1 - \frac{w_{j,fl}^{\text{ex}}}{\omega_{j,fn}} \sum_{k,m} \sum_{\eta'} \mathbb{E} [h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}] \right) \\ &\quad - \sum_n \sum_r \frac{\mathbb{E} [|s_{jr,fn}|^2]}{w_{j,fl}^{\text{ex}}} \sum_{k,m} \sum_{\eta'} \phi_{j,fn,\eta,\eta'}^2 \mathbb{E} \left[ \frac{1}{h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}} \right] \\ &\quad - \log w_{j,fl}^{\text{ex}} + \text{const}. \end{aligned} \quad (58)$$

Observing this distribution, one can see that it involves a linear term in  $\log w_{j,fl}^{\text{ex}}$ , a linear term in  $w_{j,fl}^{\text{ex}}$  and a linear term in  $\frac{1}{w_{j,fl}^{\text{ex}}}$ . The optimal approximating distribution  $q^*(w_{j,fl}^{\text{ex}})$  is hence an instance of the generalized inverse Gaussian (GIG) distribution, whose probability distribution function (PDF) is given by

$$GIG(y; \gamma, \rho, \tau) = \frac{\exp\{(\gamma - 1) \log y - \rho y - \frac{\tau}{y}\} \rho^{\frac{\gamma}{2}}}{2\tau^{\frac{\gamma}{2}} K_{\gamma}(2\sqrt{\rho\tau})}, \quad (59)$$

for  $y \geq 0$ ,  $\rho \geq 0$  and  $\tau \geq 0$ , where  $K_{\gamma}(\cdot)$  is the modified Bessel function of the second kind. The gamma distribution is a special case of the GIG distribution [4] when  $\tau = 0$  and  $\gamma > 0$ . Similarly, the inverse gamma distribution is another special case [4] when  $\rho = 0$  and  $\gamma < 0$ .

In the exponent of the PDF of the GIG distribution, we can match  $\frac{\tau}{y}$  to the first line of (58) in a ‘‘completing the square’’ fashion [2]. Similarly,  $\rho y$  is matched to the second line of (58). Finally, the last line of (58) is matched to  $(\gamma - 1) \log y$ . By doing this we obtain the following update equations for the parameter of  $q^*(w_{j,fl}^{\text{ex}})$   $\tau_{w,j,fl}^{\text{ex}}$ ,  $\rho_{w,j,fl}^{\text{ex}}$  and  $\gamma_{w,j,fl}^{\text{ex}}$



$$\tau_{w,j,fl}^{\text{ex}} = \sum_n \sum_r \mathbb{E}[|s_{jr,fn}|^2] \sum_{k,m} \sum_{\eta'} \phi_{j,fn,\eta'}^2 \mathbb{E}\left[\frac{1}{h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}}\right], \quad (60)$$

$$\rho_{w,j,fl}^{\text{ex}} = \sum_n \frac{R_j}{\omega_{j,fn}} \sum_{k,m} \sum_{\eta'} \mathbb{E}[h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}], \quad (61)$$

$$\gamma_{w,j,fl}^{\text{ex}} = 0. \quad (62)$$

Embedding the update equation for  $\phi_{j,fn,\eta'}$  given in (56) into (60), we obtain the following:

$$\begin{aligned} \tau_{w,j,fl}^{\text{ex}} &= \sum_n \left[ \left( \sum_r \mathbb{E}[|s_{jr,fn}|^2] \right) \right. \\ &\quad \left. \sum_{k,m} \sum_{\eta'} \left( \left( \frac{1}{C_{j,fn}} \mathbb{E}\left[\frac{1}{h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} w_{j,fl}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}}\right] \right)^{-1} \right)^2 \right. \\ &\quad \left. \mathbb{E}\left[\frac{1}{h_{j,c,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}}\right] \right] \\ &= \mathbb{E}\left[\frac{1}{w_{j,c,fl}^{\text{ex}}}\right]^{-2} \sum_n \left( \frac{1}{C_{j,fn}^2} \left( \sum_r \mathbb{E}[|s_{jr,fn}|^2] \right) \right. \\ &\quad \left. \sum_{k,m} \sum_{\eta'} \mathbb{E}\left[\frac{1}{h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}}\right]^{-1} \right). \end{aligned} \quad (63)$$

Finally, we can write this update equation in matrix form as shown below:

$$\begin{aligned} \tau_{w,j}^{\text{ex}} &= \mathbb{E}\left[\frac{1}{\mathbf{w}_j^{\text{ex}}}\right]^{-2} \odot \left( \left( \mathbb{E}[|\mathbf{S}_j|^2] \odot \mathbf{C}_j^{-2} \odot \mathbb{E}\left[\frac{1}{\mathbf{V}_j^{\text{ft}}}\right]^{-1} \right) \right. \\ &\quad \left. \left( \mathbb{E}\left[\frac{1}{\mathbf{U}_j^{\text{ex}}}\right]^{-1} \mathbb{E}\left[\frac{1}{\mathbf{G}_j^{\text{ex}}}\right]^{-1} \mathbb{E}\left[\frac{1}{\mathbf{H}_j^{\text{ex}}}\right]^{-1} \right)^T \right). \end{aligned} \quad (64)$$

Note that in (64), the power operations like  $\mathbf{X}^{-a}$  are element-wise operations. Furthermore, the symbol  $\odot$  means element-wise matrix multiplication.

Similarly, replacing  $\omega_{j,fn}$  in (65) with its update equation shown in (52) yields the following:

$$\rho_{w,j,fl}^{\text{ex}} = \sum_n \left( \frac{R_j}{\sum_{\eta} \sum_{\eta'} \mathbb{E}[v_{j,fn,\eta,\eta'}]} \sum_{k,m} \sum_{\eta'} \mathbb{E}[h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}] \right). \quad (65)$$

The update equation of  $\rho_{w,j}^{\text{ex}}$  is written in the matrix form as follows:

$$\rho_{w,j}^{\text{ex}} = R_j \mathbb{E}[\mathbf{V}_j^{\text{ex}}]^{-1} \left( \mathbb{E}[\mathbf{U}_j^{\text{ex}}] \mathbb{E}[\mathbf{G}_j^{\text{ex}}] \mathbb{E}[\mathbf{H}_j^{\text{ex}}] \right)^T. \quad (66)$$

For the other multilevel NMF parameters, the derivations are performed by following the same steps. Therefore, in the following, we skip the details of the derivations and give only the final update equations.

**Update Equations for  $u_{j,lk}^{\text{ex}}$ :** The update equation for  $\tau_{u,j,lk}^{\text{ex}}$  is given in the following

$$\begin{aligned} \tau_{u,j,lk}^{\text{ex}} = & \mathbb{E} \left[ \frac{1}{u_{j,lk}^{\text{ex}}} \right]^{-2} \sum_{f,n} \left( \frac{1}{C_{j,fn}^2} \sum_r \mathbb{E}[|s_{jr,fn}|^2] \right. \\ & \left. \sum_m \sum_{\eta'} \mathbb{E} \left[ \frac{1}{h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,fl}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}} \right]^{-1} \right). \end{aligned} \quad (67)$$

The matrix version of this update equation is written as

$$\begin{aligned} \boldsymbol{\tau}_{u,j}^{\text{ex}} = & \mathbb{E}_q \left[ \frac{1}{\mathbf{U}_j^{\text{ex}}} \right]^{-2} \odot \left[ \left( \mathbb{E}_q \left[ \frac{1}{\mathbf{W}_{j,c}^{\text{ex}}} \right]^{-1} \right)^T \left( \mathbb{E}[|\mathbf{S}_j|^2] \odot \mathbf{C}_j^{-2} \odot \mathbb{E} \left[ \frac{1}{\mathbf{V}_{j,c}^{\text{ft}}} \right]^{-1} \right) \right. \\ & \left. \left( \mathbb{E} \left[ \frac{1}{\mathbf{G}_{j,c}^{\text{ex}}} \right]^{-1} \mathbb{E} \left[ \frac{1}{\mathbf{H}_{j,c}^{\text{ex}}} \right]^{-1} \right)^T \right]. \end{aligned} \quad (68)$$

The update equation for  $\rho_{u,j,lk}^{\text{ex}}$  is given in the following

$$\rho_{u,j,lk}^{\text{ex}} = \sum_{f,n} \left( \frac{R_j}{\sum_{\eta} \sum_{\eta'} \mathbb{E}[v_{j,fn,\eta,\eta'}]} \sum_m \sum_{\eta'} \mathbb{E}[h_{j,mn}^{\text{ex}} g_{j,km}^{\text{ex}} u_{j,fl}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}] \right). \quad (69)$$

The matrix form is given by

$$\boldsymbol{\rho}_{u,j}^{\text{ex}} = R_j \mathbb{E}[\mathbf{W}_j]^T \mathbb{E}[\mathbf{V}_j]^{-1} \left( \mathbb{E}[\mathbf{G}_j^{\text{ex}}] \mathbb{E}[\mathbf{H}_j^{\text{ex}}] \right)^T. \quad (70)$$

Finally,

$$\gamma_{u,j,lk}^{\text{ex}} = 0. \quad (71)$$

**Update Equations for  $g_{j,km}^{\text{ex}}$ :** The update equation for  $\tau_{g,j,km}^{\text{ex}}$  is written as follows

$$\begin{aligned} \tau_{g,j,km}^{\text{ex}} = & \mathbb{E} \left[ \frac{1}{g_{j,km}^{\text{ex}}} \right]^{-2} \sum_{f,n} \left( \frac{1}{C_{j,fn}^2} \left( \sum_r \mathbb{E}[|s_{jr,fn}|^2] \right) \right. \\ & \left. \sum_l \sum_{\eta'} \mathbb{E} \left[ \frac{1}{h_{j,mn}^{\text{ex}} u_{j,lk}^{\text{ex}} w_{j,fl}^{\text{ex}} v_{j,fn,\eta'}^{\text{ft}}} \right]^{-1} \right). \end{aligned} \quad (72)$$

The matrix version is

$$\begin{aligned} \boldsymbol{\tau}_{g,j}^{\text{ex}} = & \mathbb{E} \left[ \frac{1}{\mathbf{G}_j^{\text{ex}}} \right]^{-2} \odot \left( \left( \mathbb{E} \left[ \frac{1}{\mathbf{W}_j^{\text{ex}}} \right]^{-1} \mathbb{E} \left[ \frac{1}{\mathbf{U}_j^{\text{ex}}} \right]^{-1} \right)^T \right. \\ & \left. \left( \mathbb{E}[|\mathbf{S}_j|^2] \odot \mathbf{C}_j^{-2} \odot \mathbb{E} \left[ \frac{1}{\mathbf{V}_j^{\text{ft}}} \right]^{-1} \right) \left( \mathbb{E} \left[ \frac{1}{\mathbf{H}_j^{\text{ex}}} \right]^{-1} \right)^T \right). \end{aligned} \quad (73)$$

The update equation for  $\rho_{g,j,km}^{\text{ex}}$  is as follows

$$\rho_{g,j,km}^{\text{ex}} = \sum_{f,n} \left( \frac{R_j}{\sum_{\eta} \sum_{\eta'} \mathbb{E}[v_{j,f,n,\eta,\eta'}]} \sum_l \sum_{\eta'} \mathbb{E}_q [h_{j,mn}^{\text{ex}} u_{j,lk}^{\text{ex}} w_{j,fl}^{\text{ex}} v_{j,f,n,\eta'}^{\text{ft}}] \right). \quad (74)$$

The matrix version is

$$\boldsymbol{\rho}_{g,j}^{\text{ex}} = R_j (\mathbb{E}[\mathbf{W}_j^{\text{ex}}] \mathbb{E}[\mathbf{U}_j^{\text{ex}}])^T \mathbb{E}[\mathbf{V}_j^{\text{ex}}]^{-1} \mathbb{E}[\mathbf{H}_j^{\text{ex}}]^T. \quad (75)$$

As with the above multilevel NMF parameters,

$$\gamma_{g,j,km}^{\text{ex}} = 0. \quad (76)$$

**Update Equations for  $h_{j,mn}^{\text{ex}}$  :** The update equation for  $\tau_{h,j,mn}^{\text{ex}}$  is expressed as follows

$$\tau_{h,j,mn}^{\text{ex}} = \mathbb{E} \left[ \frac{1}{h_{j,mn}^{\text{ex}}} \right]^{-2} \sum_f \left( \frac{1}{C_{j,fn}^2} \left( \sum_r \mathbb{E}[|s_{jr,fn}|^2] \right) \sum_{k,l} \sum_{\eta'} \mathbb{E} \left[ \frac{1}{g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} w_{j,fl}^{\text{ex}} v_{j,f,n,\eta'}^{\text{ft}}} \right]^{-1} \right). \quad (77)$$

The matrix version

$$\boldsymbol{\tau}_{h,j}^{\text{ex}} = \mathbb{E} \left[ \frac{1}{\mathbf{H}_j^{\text{ex}}} \right]^{-2} \odot \left( \left( \mathbb{E} \left[ \frac{1}{\mathbf{W}_j^{\text{ex}}} \right]^{-1} \mathbb{E} \left[ \frac{1}{\mathbf{U}_j^{\text{ex}}} \right]^{-1} \mathbb{E} \left[ \frac{1}{\mathbf{G}_j^{\text{ex}}} \right]^{-1} \right)^T \left( \mathbb{E}[|\mathbf{S}_j|^2] \odot \mathbf{C}_j^{-2} \odot \mathbb{E} \left[ \frac{1}{\mathbf{V}_j^{\text{ft}}} \right]^{-1} \right). \quad (78)$$

The update equation for  $\rho_{h,j,mn}^{\text{ex}}$  is as follows

$$\rho_{h,j,mn}^{\text{ex}} = \sum_{f,n} \left( \frac{R_j}{\sum_{\eta} \sum_{\eta'} \mathbb{E}[v_{j,f,n,\eta,\eta'}]} \sum_{k,l} \sum_{\eta'} \mathbb{E}[g_{j,km}^{\text{ex}} u_{j,lk}^{\text{ex}} w_{j,fl}^{\text{ex}} v_{j,f,n,\eta'}^{\text{ft}}] \right). \quad (79)$$

The matrix version is

$$\boldsymbol{\rho}_{h,j}^{\text{ex}} = R_j (\mathbb{E}[\mathbf{W}_j^{\text{ex}}] \mathbb{E}[\mathbf{U}_j^{\text{ex}}] \mathbb{E}[\mathbf{G}_j^{\text{ex}}])^T \mathbb{E}[\mathbf{V}_j^{\text{ex}}]^{-1}. \quad (80)$$

As with all the other multilevel NMF parameters,

$$\gamma_{h,j,km}^{\text{ex}} = 0. \quad (81)$$

For the filter multilevel NMF parameters, the derivation of the update equations is similar to the derivation of the excitation multilevel NMF parameters and so are the final update equations.

### 2.2.4 Variational Updates for the Source Components

The distribution  $\tilde{f}(\mathbf{X}, \mathbf{s}_{fn}, \boldsymbol{\Omega})$  of the source components  $\mathbf{s}_{fn}$  is given by

$$\begin{aligned} \log \tilde{f}(\mathbf{X}, \mathbf{Z}, \boldsymbol{\Omega})_{\mathbf{S}} &= \mathbf{s}_{fn}^H \mathbb{E}[\mathbf{A}_f^H] (\sigma_b^2 \mathbf{I})^{-1} \mathbf{x}_{fn} + \mathbf{x}_{fn}^H (\sigma_b^2 \mathbf{I})^{-1} \mathbb{E}[\mathbf{A}_f] \mathbf{s}_{fn} \\ &\quad - \frac{1}{\sigma_b^2} (\mathbf{s}_{fn}^H \mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f] \mathbf{s}_{fn}) \\ &\quad - \sum_j \sum_r |s_{jr,fn}|^2 \sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'}^2 \mathbb{E} \left[ \frac{1}{v_{j,fn,\eta,\eta'}} \right] + \text{const.} \end{aligned} \quad (82)$$

Replacing  $\phi_{j,fn,\eta,\eta'}$  with its value shown in (56) yields

$$\begin{aligned} \log \tilde{f}(\mathbf{X}, \mathbf{Z}, \boldsymbol{\Omega})_{\mathbf{S}} &= \mathbf{s}_{fn}^H \mathbb{E}[\mathbf{A}_f^H] (\sigma_b^2 \mathbf{I})^{-1} \mathbf{x}_{fn} + \mathbf{x}_{fn}^H (\sigma_b^2 \mathbf{I})^{-1} \mathbb{E}[\mathbf{A}_f] \mathbf{s}_{fn} \\ &\quad - \frac{1}{\sigma_b^2} (\mathbf{s}_{fn}^H \mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f] \mathbf{s}_{fn}) \\ &\quad - \mathbf{s}_{fn}^H \mathbf{C}_{fn}^{-1} \mathbf{s}_{fn} + \text{const}, \end{aligned} \quad (83)$$

where  $\mathbf{C}_{fn}^{-1} = \text{diag}(C_{j,fn}^{-1})_{r=1}^R$  is a diagonal matrix with the main diagonal containing the normalization factor  $C_{j,fn}^{-1}$  repeated  $R_j$  times for each  $j$ .

This distribution involves a linear term in  $\mathbf{s}_{fn}$ , its conjugate, and quadratic terms. The optimal approximating distribution is thus a Gaussian given by

$$\mathbf{s}_{fn} \sim \mathcal{N}(\boldsymbol{\mu}_{\mathbf{s},fn}, \mathbf{R}_{\mathbf{ss},fn}). \quad (84)$$

By ‘‘completing the square’’ wrt.  $\boldsymbol{\mu}_{\mathbf{s},fn}$  and  $\mathbf{R}_{\mathbf{ss},fn}$  in (83) we derive the update equations for these two parameters. First we derive the update equation of the covariance. For this, we rearrange the quadratic terms make them equal to  $-\mathbf{s}_{fn}^H \mathbf{R}_{\mathbf{ss},fn}^{-1} \mathbf{s}_{fn}$ . By doing this we obtain the covariance given in the following

$$\begin{aligned} \mathbf{R}_{\mathbf{ss},fn} &= (\mathbf{C}_{fn}^{-1} + (\sigma_b^2 \mathbf{I})^{-1} \mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f])^{-1} \\ &= \mathbf{C}_{fn} - \mathbf{C}_{fn} (\sigma_b^2 \mathbf{I} + \mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f] \mathbf{C}_{fn})^{-1} \mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f] \mathbf{C}_{fn}, \end{aligned} \quad (85)$$

Note that we used the Woodbury matrix identity [2] for the inversion here. Similarly for the update equation of the mean, we arrange the linear terms of the mean and make them equal to  $\mathbf{s}_{fn}^H \mathbf{R}_{\mathbf{ss},fn}^{-1} \boldsymbol{\mu}_{\mathbf{s},fn} + \boldsymbol{\mu}_{\mathbf{s},fn}^H \mathbf{R}_{\mathbf{ss},fn}^{-1} \mathbf{s}_{fn}$ . This yields the following update equation for the mean

$$\boldsymbol{\mu}_{\mathbf{s},fn} = \mathbf{R}_{\mathbf{ss},fn} \mathbb{E}[\mathbf{A}_f^H] (\sigma_b^2 \mathbf{I})^{-1} \mathbf{x}_{fn}. \quad (86)$$

### 2.2.5 Variational Updates for the Mixing Parameters

The distribution  $\tilde{f}(\mathbf{X}, \underline{\mathbf{A}}_f, \boldsymbol{\Omega})$  of the reshaped mixing parameters  $\underline{\mathbf{A}}_f$  is given by

$$\begin{aligned}
\log \tilde{f}(\mathbf{X}, \underline{\mathbf{A}}_f, \Omega) &= -\underline{\mathbf{A}}_f^H \frac{1}{\sigma_b^2} \sum_n \text{diag}(\underbrace{\mathbf{R}_{\mathbf{s},fn}^T, \dots, \mathbf{R}_{\mathbf{s},fn}^T}_{I \text{ times}}) \underline{\mathbf{A}}_f \\
&\quad + \underline{\mathbf{A}}_f^H \frac{1}{\sigma_b^2} \sum_n \mathbf{R}_{\mathbf{x}\mathbf{s},fn} + \frac{1}{\sigma_b^2} \left( \sum_n \mathbf{R}_{\mathbf{x}\mathbf{s},fn}^H \right) \underline{\mathbf{A}}_f \\
&\quad + \text{const}, \tag{87}
\end{aligned}$$

where  $\mathbf{R}_{\mathbf{s},fn}$  is the second raw moment of the source coefficients and is given by

$$\mathbf{R}_{\mathbf{s},fn} = \boldsymbol{\mu}_{\mathbf{s},nf} \boldsymbol{\mu}_{\mathbf{s},nf}^H + \mathbf{R}_{\mathbf{ss},fn}. \tag{88}$$

Similarly,  $\mathbf{R}_{\mathbf{x}\mathbf{s},fn}$  is given by

$$\mathbf{R}_{\mathbf{x}\mathbf{s},fn} = [x_{1,fn} \boldsymbol{\mu}_{\mathbf{s},fn}^H, \dots, x_{I,fn} \boldsymbol{\mu}_{\mathbf{s},fn}^H]^T. \tag{89}$$

Note that the contribution of the prior distribution vanishes, because we assumed a flat prior. Also note that due to the reshaping of the mixing matrix  $\mathbf{A}_f$  into a vector  $\underline{\mathbf{A}}_f$ , matrix multiplications *e.g.*  $\mathbf{A}_f \mathbf{s}_{fn}$  became multiplications of two vectors. As a result of the dimensionality mismatch the vector multiplication cannot be performed anymore. Note that in the given example each row of the mixing matrix, which correspond to each channel of the mixture respectively is multiplied by the source. Therefore, we define the term  $\text{diag}(\underbrace{\mathbf{R}_{\mathbf{s},fn}^T, \dots, \mathbf{R}_{\mathbf{s},fn}^T}_{I \text{ times}})$

indicating a block diagonal matrix, where  $\mathbf{R}_{\mathbf{s},fn}$  is repeated on the diagonal  $I$  times. Similarly,  $\mathbf{R}_{\mathbf{x}\mathbf{s},fn}$  is composed of multiplying  $\boldsymbol{\mu}_{\mathbf{s},fn}^H$  with each channel of the mixture.

The distribution given in (87) involves a linear term in  $\underline{\mathbf{A}}_f$ , its conjugate, and a quadratic term. Hence, the optimal approximating distribution is a Gaussian given by

$$\underline{\mathbf{A}}_f \sim \mathcal{N}(\boldsymbol{\mu}_{\underline{\mathbf{A}},f}, \mathbf{R}_{\underline{\mathbf{A}}\underline{\mathbf{A}},f}). \tag{90}$$

By “completing the square” wrt.  $\boldsymbol{\mu}_{\underline{\mathbf{A}},f}$  and  $\mathbf{R}_{\underline{\mathbf{A}}\underline{\mathbf{A}},f}$  in (87) we derive the update equations for these two parameters. First we derive the update equation of the covariance. For this, we rearrange the quadratic terms make them equal to  $-\underline{\mathbf{A}}_f^H \mathbf{R}_{\underline{\mathbf{A}}\underline{\mathbf{A}},f}^{-1} \underline{\mathbf{A}}_f$ . By doing this we obtain the covariance given in the following

$$\mathbf{R}_{\underline{\mathbf{A}}\underline{\mathbf{A}},f} = \left( \frac{1}{\sigma_b^2} \sum_n \text{diag}(\underbrace{\mathbf{R}_{\mathbf{s},fn}^T, \dots, \mathbf{R}_{\mathbf{s},fn}^T}_{I \text{ times}}) \right)^{-1}, \tag{91}$$

Similarly, for the mean, we rearrange the linear terms and make them equal to  $\underline{\mathbf{A}}_f^H \mathbf{R}_{\underline{\mathbf{A}}\underline{\mathbf{A}},f}^{-1} \boldsymbol{\mu}_{\underline{\mathbf{A}},f} + \boldsymbol{\mu}_{\underline{\mathbf{A}},f}^H \mathbf{R}_{\underline{\mathbf{A}}\underline{\mathbf{A}},f}^{-1} \underline{\mathbf{A}}_f$  which yields

$$\boldsymbol{\mu}_{\underline{\mathbf{A}},f} = \mathbf{R}_{\underline{\mathbf{A}}\underline{\mathbf{A}},f} \frac{1}{\sigma_b^2} \sum_n \mathbf{R}_{\mathbf{x}\mathbf{s},fn}, \tag{92}$$

### 2.3 Computation of the Expectations Involved in the Updates

The update equations for the approximating distributions require the evaluation of some expectations. These expectations are to be evaluated with respect to the other distributions. Therefore an iterative update procedure similar to the Expectation-Maximization (E-M) algorithm is followed. In the variational E-step, these expectations are calculated. In the variational M-step, the approximating distributions are re-calculated with the new expectation values.

The expectations related to the generalized inverse Gaussian distribution include  $\mathbb{E}[y]$  and  $\mathbb{E}[\frac{1}{y}]$ . These expectations are computed using the following two formulae [4]:

$$\mathbb{E}[y] = \frac{\mathcal{K}_{\gamma+1}(2\sqrt{\rho\tau})\sqrt{\tau}}{\mathcal{K}_{\gamma}(2\sqrt{\rho\tau})\sqrt{\rho}}, \quad (93)$$

$$\mathbb{E}[\frac{1}{y}] = \frac{\mathcal{K}_{\gamma-1}(2\sqrt{\rho\tau})\sqrt{\rho}}{\mathcal{K}_{\gamma}(2\sqrt{\rho\tau})\sqrt{\tau}}. \quad (94)$$

We remind you that the multilevel NMF parameters can be fixed or adapted to the data. The expectations are only calculated for the adapted multilevel NMF parameters.

Recall that we reshaped the mixing matrix into a vector and calculated the optimal actor for the distribution we defined for the vector form mixing system. Hence, we have  $\mathbb{E}[\underline{\mathbf{A}}_f \underline{\mathbf{A}}_f^H]$  and  $\mathbb{E}[\underline{\mathbf{A}}_f]$ . However in (85), we need to calculate  $\mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f]$ . Therefore, we need to reshape the mixing parameters into a matrix and consider the interchannel relationships within the mixing matrix to calculate the expectations. Hence, the expectation  $(\mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f])_{(jj')}$  is given by

$$\mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f]_{jj'} = \mathbb{E}\left[\sum_i a_{ji}^H a_{ij'}\right], \quad (95)$$

where  $(\cdot)_{(jj')}$  indicates the expectation between the mixing parameters corresponding to the sources  $(j, j')$ . Note that for this, we make use of the linearity of the expectation operator, namely  $\mathbb{E}[a\mathbf{X} + b\mathbf{Y}] = a\mathbb{E}[\mathbf{X}] + b\mathbb{E}[\mathbf{Y}]$ . So, we consider the expectation matrix  $\mathbb{E}[\underline{\mathbf{A}}_f \underline{\mathbf{A}}_f^H]$  as a block matrix and basically add up the diagonal blocks to reestablish the interchannel relationships to calculate  $\mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f]$  as shown

$$\mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f] = \sum_i \left( \left[ \mathbb{E}[\underline{\mathbf{A}}_f \underline{\mathbf{A}}_f^H] \right]_{ii} \right)^T, \quad (96)$$

where  $[\cdot]_{ii}$  indicates the  $R \times R$  diagonal block corresponding to the channel  $i$  and

$$\mathbb{E}[\underline{\mathbf{A}}_f \underline{\mathbf{A}}_f^H] = \underline{\boldsymbol{\mu}}_{\underline{\mathbf{A}},f} \underline{\boldsymbol{\mu}}_{\underline{\mathbf{A}},f}^H + \mathbf{R}_{\underline{\mathbf{A}},f}. \quad (97)$$

Similarly, in (86), we need to calculate  $\mathbb{E}[\mathbf{A}_f^H]$ . For this, we only need to reshape the expectation  $\underline{\boldsymbol{\mu}}_{\underline{\mathbf{A}},f}^H$  back into a matrix

$$\mathbb{E}[\mathbf{A}_f^H]_{i,1\dots R} = (\underline{\boldsymbol{\mu}}_{\underline{\mathbf{A}},f})_{((i-1)R+1,\dots,iR)}^H. \quad (98)$$

## 2.4 Lower Bound

We calculate the new lower bound  $\mathcal{B}(q)$  after each M-step. Here we compare the new lower bound with the previous one and set a termination condition according to this change. The lower bound should never decrease. This fact enables us to check the update equations and their implementation for their correctness. In general, if the increase in the lower bound is insignificant compared to previous iterations, we stop. The lower bound has already been defined in the following

$$\begin{aligned}
\mathcal{B}(q) &= \mathbb{E}[\log p(\mathbf{X}|\mathbf{S}, \mathbf{A})] \\
&+ \mathbb{E}\left[-F \cdot N \cdot R \cdot \log \pi\right. \\
&+ \sum_{j,fn} R_j \left(-\log \omega_{j,fn} + 1 - \frac{1}{\omega_{j,fn}} \sum_{\eta} \sum_{\eta'} v_{j,fn,\eta,\eta'}\right) \\
&+ \left. \sum_{j,fn} \sum_r -|s_{jr,fn}|^2 \sum_{\eta} \sum_{\eta'} \phi_{j,fn,\eta,\eta'}^2 \frac{1}{v_{j,fn,\eta,\eta'}}\right] \\
&- \mathbb{E}[\log q(\mathbf{S})] \\
&+ \mathbb{E}[\log p(\mathbf{A})] - \mathbb{E}[\log q(\mathbf{A})] \\
&+ \mathbb{E}[\log p(\mathbf{W}^{\text{ex}})] - \mathbb{E}[\log q(\mathbf{W}^{\text{ex}})] \\
&+ \mathbb{E}[\log p(\mathbf{W}^{\text{ft}})] - \mathbb{E}[\log q(\mathbf{W}^{\text{ft}})] \\
&+ \mathbb{E}[\log p(\mathbf{U}^{\text{ex}})] - \mathbb{E}[\log q(\mathbf{U}^{\text{ex}})] \\
&+ \mathbb{E}[\log p(\mathbf{U}^{\text{ft}})] - \mathbb{E}[\log q(\mathbf{U}^{\text{ft}})] \\
&+ \mathbb{E}[\log p(\mathbf{G}^{\text{ex}})] - \mathbb{E}[\log q(\mathbf{G}^{\text{ex}})] \\
&+ \mathbb{E}[\log p(\mathbf{G}^{\text{ft}})] - \mathbb{E}[\log q(\mathbf{G}^{\text{ft}})] \\
&+ \mathbb{E}[\log p(\mathbf{H}^{\text{ex}})] - \mathbb{E}[\log q(\mathbf{H}^{\text{ex}})] \\
&+ \mathbb{E}[\log p(\mathbf{H}^{\text{ft}})] - \mathbb{E}[\log q(\mathbf{H}^{\text{ft}})]. \tag{99}
\end{aligned}$$

Note that for  $\mathbb{E}[p(\mathbf{S}|\mathbf{V})]$  we used the approximation we derived which is shown in (50).

Also note that for all the variational variables, the expectations of the log of the approximating  $q$  distributions correspond to their negative entropies. Note also that the lower bound consists of the the expectation of the logarithm of the prior distribution ( $p$  distribution) minus the expectation of the logarithm of the variational distribution ( $q$  distribution) pairs except for the log-likelihood. For the log-likelihood, we calculate the expectation as follows

$$\begin{aligned}
\mathbb{E}[\log p(\mathbf{X}|\mathbf{S}, \mathbf{A})] &= \mathbb{E}\left[\sum_{f,n} \log \mathcal{N}(\mathbf{x}_{fn}|\mathbf{A}_f \mathbf{s}_{fn}, \sigma_b^2 \mathbf{I})\right], \\
&= -\sum_{f,n} \left(\log \pi \sigma_b^2 + \frac{1}{\sigma_b^2} \mathbb{E}[(\mathbf{x}_{fn} - \mathbf{A}_f \mathbf{s}_{fn})^H (\mathbf{x}_{fn} - \mathbf{A}_f \mathbf{s}_{fn})]\right), \\
&= -\sum_{f,n} \left(\log \pi \sigma_b^2 + \frac{1}{\sigma_b^2} (\mathbf{x}_{fn}^H \mathbf{x}_{fn} - \mathbf{x}_{fn}^H \mathbb{E}[\mathbf{A}_f] \mathbb{E}[\mathbf{s}_{fn}] \right. \\
&\quad \left. - \mathbb{E}[\mathbf{s}_{fn}^H] \mathbb{E}[\mathbf{A}_f^H] \mathbf{x}_{fn} + \mathbb{E}[\mathbf{s}_{fn}^H (\mathbf{A}_f)^H \mathbf{A}_f \mathbf{s}_{fn}])\right), \\
&= -\sum_{f,n} \log \pi \sigma_b^2 + \frac{1}{\sigma_b^2} (\mathbf{x}_{fn}^H \mathbf{x}_{fn} - \mathbf{x}_{fn}^H \boldsymbol{\mu}_{\mathbf{A},f} \boldsymbol{\mu}_{\mathbf{s},fn} - \boldsymbol{\mu}_{\mathbf{s},fn}^H \boldsymbol{\mu}_{\mathbf{A},f}^H \mathbf{x}_{fn} \\
&\quad + \text{tr}(\mathbb{E}[\mathbf{s}_{fn} \mathbf{s}_{fn}^H] \mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f])), \\
&= -F \cdot N \cdot I \cdot \log \pi \sigma_b^2 - \sum_{f,n} \frac{1}{\sigma_b^2} \left( \mathbf{x}_{fn}^H \mathbf{x}_{fn} - \mathbf{x}_{fn}^H \boldsymbol{\mu}_{\mathbf{A},f} \boldsymbol{\mu}_{\mathbf{s},fn} \right. \\
&\quad \left. - \boldsymbol{\mu}_{\mathbf{s},fn}^H \boldsymbol{\mu}_{\mathbf{A},f}^H \mathbf{x}_{fn} + \text{tr}((\boldsymbol{\mu}_{\mathbf{s},fn} \boldsymbol{\mu}_{\mathbf{s},fn}^H + \mathbf{R}_{\mathbf{ss},fn})(\mathbb{E}[\mathbf{A}_f^H \mathbf{A}_f])) \right). \tag{100}
\end{aligned}$$

For the expectation of the approximation of  $p(\mathbf{S}|\mathbf{V})$ , –the second, third and fourth lines of (99)– we first replace the auxiliary variables with their values given in (52, 56) as follows

$$\begin{aligned}
\mathbb{E}[p(\mathbf{S}|\mathbf{V})] &\geq -F \cdot N \cdot R \cdot \log \pi \\
&\quad + \sum_{j,fn} R_j \left( -\log \left( \sum_{\eta} \sum_{\eta'} \mathbb{E}[v_{j,fn,\eta,\eta'}] \right) \right) \\
&\quad - \sum_{j,fn} \sum_r \mathbb{E}[|s_{jr,fn}|^2] \frac{1}{\sum_{\eta} \sum_{\eta'} \mathbb{E}\left[\frac{1}{v_{j,fn,\eta,\eta'}}\right]^{-1}}
\end{aligned}$$

Due to the factorization given in (42), the expectations  $\mathbb{E}[v_{j,fn,\eta,\eta'}]$  and  $\mathbb{E}\left[\frac{1}{v_{j,fn,\eta,\eta'}}\right]$  are computed for each multilevel NMF component individually as given in (93, 94). Furthermore, the expectation  $\mathbb{E}[|s_{jr,fn}|^2]$  is the second raw moment of source component  $s_{jr,fn}$  and is computed using (88).

The expectation of the logarithm of the optimal approximating distribution of the source components  $q(\mathbf{S})$  is given by

$$\begin{aligned}
-\mathbb{E}[\log q(\mathbf{S})] &= -\sum_{fn} \mathbb{E}[\log \mathcal{N}(\mathbf{s}_{fn}|\boldsymbol{\mu}_{\mathbf{s},fn}, \mathbf{R}_{\mathbf{ss},fn})], \\
&= \sum_{fn} \log\{(\pi e)^R \det(\mathbf{R}_{\mathbf{ss},fn})\}. \tag{101}
\end{aligned}$$

About the mixing matrix, we remind you that the prior distribution of the mixing coefficients does not contribute to the lower bound, because it is flat. The expectation of the optimal approximating distribution of the mixing coefficients is given by



$$\begin{aligned}
\mathbb{E}[\log p(\underline{\mathbf{A}})] - \mathbb{E}[\log q(\underline{\mathbf{A}})] &= - \sum_f \mathbb{E}[\ln \mathcal{N}(\underline{\mathbf{A}}_f | \boldsymbol{\mu}_{\underline{\mathbf{A}},f}, \mathbf{R}_{\underline{\mathbf{A}},f})], \\
&= \sum_f \log\{(\pi e)^{2R} \det(\mathbf{R}_{\underline{\mathbf{A}},f})\}. \quad (102)
\end{aligned}$$

Finally, for one of the multilevel NMF parameters, *e.g.* for  $w_{j,c,fl}^{\text{ex}}$ , this pair writes as follows:

$$\begin{aligned}
\mathbb{E}_q[\log p(w_{j,c,fl}^{\text{ex}})] - \mathbb{E}_q[\log q(w_{j,c,fl}^{\text{ex}})] &= \rho_{w,j,c,fl}^{\text{ex}} \mathbb{E}_q[w_{j,c,fl}^{\text{ex}}] + \tau_{w,j,c,fl}^{\text{ex}} \mathbb{E}_q\left[\frac{1}{w_{j,c,fl}^{\text{ex}}}\right] \\
&\quad + \log \mathcal{K}_{\gamma_{w,j,c,fl}^{\text{ex}}}(2\sqrt{\rho\tau}) + \ln 2 \\
&\quad - \frac{\gamma_{w,j,c,fl}^{\text{ex}}}{2} (\ln \rho_{w,j,c,fl}^{\text{ex}} - \ln \tau_{w,j,c,fl}^{\text{ex}}). \quad (103)
\end{aligned}$$

Note that for  $\gamma_{w,j,c,fl}^{\text{ex}} = 0$ , the third line of this equation disappears. The calculation of the contribution of the other multilevel NMF parameters to the lower bound is calculated similarly as given in (103).

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35042 Rennes Cedex

Publisher  
Inria  
Domaine de Volveau - Rocquencourt  
BP 105 - 78153 Le Chesnay Cedex  
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ISSN 0249-0803