

Bayesian Source Separation: Beyond PCA and ICA

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Abstract. Blind source separation (BSS) has become one of the major signal and image processing area in many applications. Principal component analysis (PCA) and Independent component analysis (ICA) have become two main classical approaches for this problem. However, these two approaches have their limits which are mainly, the assumptions that the data are temporally iid and that the model is exact (no noise). In this paper, we first show that the Bayesian inference framework gives the possibility to go beyond these limits while obtaining PCA and ICA algorithms as particular cases. Then, we propose different a priori models for sources which progressively account for different properties of the sources. Finally, we illustrate the application of these different models in spectrometry, in astrophysical imaging, in satellite imaging and in hyperspectral imaging.

1 Introduction

Even if PCA and ICA have their origin in data analysis [1], they have become two main classical approaches for blind source separation problem which can be presented as :

$$\mathbf{x}(t) = \mathbf{A}\mathbf{s}(t) + \boldsymbol{\epsilon}(t), \quad (1)$$

where $\mathbf{x}(t) = [x_1(t), \dots, x_m(t)]'$ is the observed vector of data, \mathbf{A} the mixing matrix, $\mathbf{s}(t) = [s_1(t), \dots, s_n(t)]'$ the sources and $\boldsymbol{\epsilon}(t) = [\epsilon_1(t), \dots, \epsilon_m(t)]'$ represents all the uncertainties (modeling uncertainty and measurement noise). t represents either time, frequency, pixel position or index number of a coefficient in a transform domain such as Fourier, spline or wavelet domain. The main problem is the estimation of the mixing matrix \mathbf{A} and the sources $\mathbf{s}(t)$.

1.1 PCA and ICA

One of the main hypothesis in PCA and ICA approaches is that the data are temporally iid, in such a way that, the time index t can be omitted. The second main hypothesis is that the observation model is exact (no noise). With these two hypotheses, we have

$$\mathbf{x} = \mathbf{A}\mathbf{s}. \quad (2)$$

All probabilistic methods are based on trying to assign or to model the probability law of the sources $p(\mathbf{s})$ and consequently $p(\mathbf{x})$. PCA based methods use only the second order statistics. The main hypothesis is $\mathbf{R}_s = \text{cov}[\mathbf{s}]$ is diagonal. Then, assuming $\mathbf{x} = \mathbf{A}\mathbf{s}$, we have $\mathbf{R}_x = \text{cov}[\mathbf{x}] = \mathbf{A}\mathbf{R}_s\mathbf{A}^t$. Thus, the PCA

algorithm, starts by estimating $\text{cov}[\mathbf{x}]$ from the data and then using the SVD, the mixing matrix \mathbf{A} can be determined up to a rotation. It is also easy to see that the PCA solution is the maximum likelihood solution :

$$\hat{\mathbf{A}} = \arg \max_{\mathbf{A}} \{p(\mathbf{x}|\mathbf{A})\} = \arg \min_{\mathbf{A}} \{-\ln p(\mathbf{x}|\mathbf{A})\} \quad (3)$$

assuming the sources are uncorrelated Gaussian :

$$p(\mathbf{s}) = \mathcal{N}(\mathbf{0}, \mathbf{R}_s) \longrightarrow p(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \mathbf{A}\mathbf{R}_s\mathbf{A}^t).$$

This can easily be seen if we note that

$$-\ln p(\mathbf{x}|\mathbf{A}) = \frac{n}{2}(\ln(2\pi) + \ln|\mathbf{A}|) + \frac{1}{2}\mathbf{x}^t(\mathbf{A}\mathbf{R}_s\mathbf{A}^t)^{-1}\mathbf{x}$$

In ICA, the main idea is to form an auxiliary vector $\mathbf{y} = \mathbf{B}\mathbf{x}$ and then determine the vector \mathbf{y} which has the most independent components, for example by

$$\hat{\mathbf{B}} = \arg \max_{\mathbf{B}} \left\{ \text{KL}(p(\mathbf{y}) : \prod_i p_{y_i}(y_i)) \right\} \quad (4)$$

where $\text{KL}(p, q)$ is the Kullback-Leibler distance or the mutual information between two probability laws p and q .

The main point is then to choose $\mathbf{y} = \hat{\mathbf{B}}\mathbf{x}$ as an estimate of \mathbf{s} . It is not too difficult to show that, if \mathbf{A} is invertible and if $\hat{\mathbf{B}} = \mathbf{A}^{-1}$, then $\mathbf{y} = \hat{\mathbf{B}}\mathbf{x} = \hat{\mathbf{B}}\mathbf{A}\mathbf{s} = \mathbf{s}$. But, can we say anything about the relation between \mathbf{s} and \mathbf{y} if the matrix is singular or if we now that the data are noisy ?

It is also interesting to note that, when \mathbf{A} is invertible, the solution obtained by the relation (4) is, mathematically, the same as the ML solution (3) when replacing \mathbf{A} by \mathbf{B}^{-1} , i.e.

$$\hat{\mathbf{B}} = \arg \max_{\mathbf{B}} \{p(\mathbf{x}|\mathbf{B})\} = \arg \min_{\mathbf{B}} \{-\ln p(\mathbf{x}|\mathbf{B})\}$$

This interpretation gives also the interesting point which is that ICA extends the PCA to the case of non Gaussian signals.

One more remark is that to obtain an explicit expression for the mutual information criterion, we need to make more assumptions about $p(\mathbf{y})$ and consequently about $p(\mathbf{x})$ and thus about $p(\mathbf{s})$. For example, if we limit our analysis to the second order statistics, we obtain PCA and if we go farther, we obtain all the HOS algorithms, and if we do any approximation for the expression of $p(\mathbf{s})$ by troncation of its development in Taylor's series, we obtain the ICA algorithms based on the contrast functions [2, 3, 4, 5, 6, 7].

2 Bayesian approach

In the Bayesian approach, we start by accounting explicitly for the errors in modeling and the noise. The simplest model is then assuming the errors to be

additive $\mathbf{x} = \mathbf{A}\mathbf{s} + \boldsymbol{\epsilon}$. Then, we assign a probability law to $\boldsymbol{\epsilon}$ to translate our prior knowledge about it. The simplest choice is to assume $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{R}_\epsilon)$ with $\mathbf{R}_\epsilon = \text{diag}[\sigma_{\epsilon_i}^2, i = 1, \dots, M]$. Then:

$$p(\mathbf{x}|\mathbf{A}, \mathbf{s}) = \mathcal{N}(\mathbf{A}\mathbf{s}, \mathbf{R}_\epsilon) \quad (5)$$

The next step is to assign $p(\mathbf{s})$ which gives the possibility to derive the joint pdf $p(\mathbf{x}, \mathbf{s}|\mathbf{A}) = p(\mathbf{x}|\mathbf{A}, \mathbf{s})p(\mathbf{s})$ and the marginal pdf

$$p(\mathbf{x}|\mathbf{A}) = \int p(\mathbf{x}|\mathbf{A}, \mathbf{s})p(\mathbf{s}) \, d\mathbf{s}. \quad (6)$$

We can then stop here and look for the Maximum likelihood (ML) solution

$$\hat{\mathbf{A}} = \arg \max_{\mathbf{A}} \{p(\mathbf{x}|\mathbf{A})\} = \arg \min_{\mathbf{A}} \{-\ln p(\mathbf{x}|\mathbf{A})\} \quad (7)$$

either directly when it is possible to obtain an analytical expression for $p(\mathbf{x}|\mathbf{A})$ as is the case of Gaussian hypothesis for $p(\mathbf{s})$, or using the EM algorithm to obtain the solution.

The interesting point is that, by this approach, we obtain the PCA and ICA methods as particular case in the limiting case of no noise ($\boldsymbol{\epsilon} = \mathbf{0}$) and invertible mixing matrix \mathbf{A} .

But, now, we can go farther. For example, if $p(\mathbf{s})$ depends on a set of unknown parameters $\boldsymbol{\theta}$ and if $p(\mathbf{x}|\mathbf{A}, \mathbf{s})$ depends on a set of unknown parameters (for example the \mathbf{R}_ϵ), then we can write the joint pdf $p(\mathbf{x}, \mathbf{s}|\mathbf{A}, \boldsymbol{\theta}, \mathbf{R}_\epsilon) = p(\mathbf{x}|\mathbf{A}, \mathbf{s}, \mathbf{R}_\epsilon)p(\mathbf{s}|\boldsymbol{\theta})$ and the marginal pdf $p(\mathbf{x}|\mathbf{A}, \boldsymbol{\theta}, \mathbf{R}_\epsilon)$ and then estimate them jointly by

$$(\hat{\mathbf{A}}, \hat{\boldsymbol{\theta}}, \hat{\mathbf{R}}_\epsilon) = \arg \max_{\mathbf{A}, \boldsymbol{\theta}, \mathbf{R}_\epsilon} \{p(\mathbf{x}|\mathbf{A}, \boldsymbol{\theta}, \mathbf{R}_\epsilon)\} \quad (8)$$

But, we can still do better, by assigning appropriate priors to obtain an expression for the joint posterior of all the unknowns

$$p(\mathbf{s}, \mathbf{A}, \boldsymbol{\theta}, \mathbf{R}_\epsilon|\mathbf{x}) \propto p(\mathbf{x}|\mathbf{A}, \mathbf{s}, \mathbf{R}_\epsilon)p(\mathbf{s}|\boldsymbol{\theta})p(\mathbf{A})p(\boldsymbol{\theta})p(\mathbf{R}_\epsilon) \quad (9)$$

from which we can infer on all the unknowns at the same time. However, this needs to assign the appropriate priors $p(\mathbf{A})$, $p(\boldsymbol{\theta})$ and $p(\mathbf{R}_\epsilon)$. There are many works on this subjects. Sometimes they can really represent our prior knowledge based on the physics of the data measurement system [8, 9], but sometimes they can only represent a mathematical tool to eliminate the degeneracy of the likelihood based criteria [10, 11, 12, 13, 14, 15].

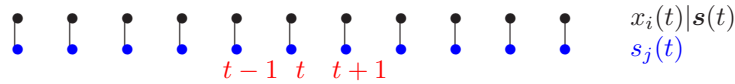
3 Proposed a priori sources models

3.1 Classical i.i.d. models

The main step in any classical Maximum likelihood (ML) or Bayesian approach is the prior modeling of the sources. Two main classes of prior models are the Generalized Gaussians (GG) and Mixture of Gaussians (MoG). The GG model

$$p(s_j) \propto \exp -\beta_j |s_j|^{\gamma_j} \quad (10)$$

has been used mainly to model the sparse sources. Many other non Gaussian prior laws have also been used. All these simple and direct models can be represented in the following scheme:



Model 1: The iid model for the sources.

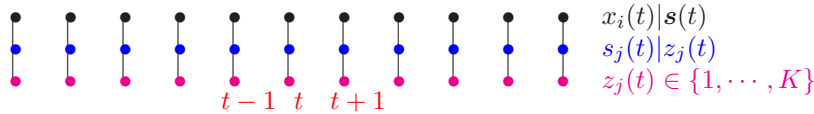
Another interesting model used frequently is the MoG:

$$p(s_j) = \sum_{k=1}^K \alpha_{j_k} \mathcal{N}(m_{j_k}, \sigma_{j_k}^2) \quad (11)$$

The interesting point in this model is in the fact that it can be described via a hidden discrete valued variable z_j in a hierarchical way

$$p(s_j|z_j = k) = \mathcal{N}(m_{j_k}, \sigma_{j_k}^2) \text{ with } P(z_j = k) = \alpha_{j_k} \quad (12)$$

This interpretation of the MoG model can be illustrated by the following scheme:

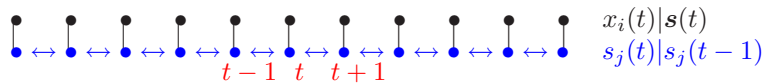


Model 2: A three level iid model for sources with an iid hidden variable $z_j(t)$. This model is equivalent to **Model 1** with a mixture of Gaussians (MoG) prior law for sources.

3.2 Markovian models accounting for time evolution

We remember that, we omitted the time index t from the equation (1), because, in all the previous cases, we assumed the sources and thus the data to be temporally iid. Now, we are going to relax this unrealistic hypothesis. Indeed, we are going to explicitly account for this time evolution.

An easy and explicit way is to model directly the sources by using a Markovian model which accounts for local dependency of the sources at time t and $t - 1$.



Model 3: A simple Markovian model for the sources.

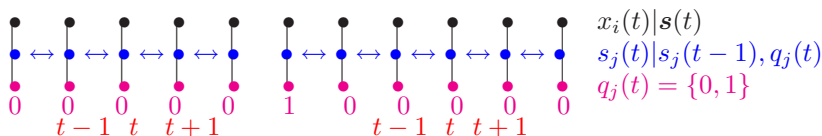
In this case, if the expression of $p(s_j(t)|s_j(t-1))$ has the parameters θ_j which are independent of time, we will have a stationnary process. There are also models in which these parameters are allowed to vary during the time allowing

to account for non stationarity of the sources. In particular, we may mention the Gauss-Markov models where

$$p(s_j(t)|s_j(t-1)) = \mathcal{N}(s_j(t-1), \theta_j(t)) \quad (13)$$

where $\theta_j(t)$ is linked to the power spectra of the sources [16, 17, 18, 19, 20, 21, 22].

Another easy and explicit way which also has the possibility to account for non stationarity of the time evolution and in particular the discontinuities in the sources is the following:



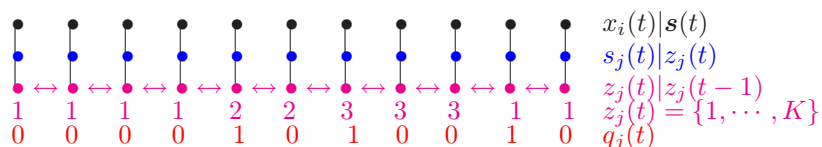
Model 4: A composite Markovian model with hidden contours variables $q_j(t)$.

In this model the binary valued hidden variable $q_j(t)$ represents the discontinuities (contours). The expression of $p(s_j(t)|s_j(t-1))$ depends on $q_j(t)$, for example:

$$\begin{aligned} p(s_j(t)|s_j(t-1), q_j(t) = 0) &= \mathcal{N}(m_{j_k}, v_{j_k}) \\ p(s_j(t)|s_j(t-1), q_j(t) = 1) &= \mathcal{N}(s_j(t-1), v_{j_k}) \end{aligned}$$

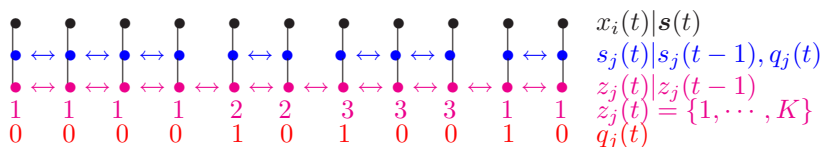
which results to $p(s_j(t)|s_j(t-1)) = (1 - \lambda_j)\mathcal{N}(m_{j_k}, v_{j_k}) + \lambda_j\mathcal{N}(s_j(t-1), v_{j_k})$ with $\lambda_j = P(q_j = 1)$.

Still another easy and explicit way which also has the possibility to account for non stationarity of the time evolution and in particular the notion of piecewise homogeneity in the sources is the following:



Model 5: A composite Markovian model with hidden classification variables $z_j(t)$. Note that $s_j(t)|z_j(t)$ are iid, but $z_j(t)$ are markovian (Potts). Note also that the contour variables $q_j(t)$ are obtained in a deterministic way from $z_j(t)$, i.e. $q_j(t) = 1 - \delta(z_j(t) - z_j(t-1))$. These contours are closed by construction.

Finally, the following model combines both **Model 3:** and **Model 5:** which gives the possibility to have a local dependency inside a region.



Model 6: A doubly Markovian model with hidden Potts variables.

4 Bayesian estimation computation

In all these models, we have to assign the prior laws:

— $p(\mathbf{x}(t)|\mathbf{s}(t), \mathbf{A}, \mathbf{R}_\epsilon)$: For this, we use the observation model (1) and assume that the noises $\epsilon_i(t)$ are centered, white, Gaussians and mutually independent. This then leads to:

$$p(\mathbf{x}(t)|\mathbf{s}(t), \mathbf{A}, \mathbf{R}_\epsilon) = \mathcal{N}(\mathbf{A}\mathbf{s}(t), \mathbf{R}_\epsilon)$$

with $\mathbf{R}_\epsilon = \text{diag} [\sigma_{\epsilon_1}^2, \dots, \sigma_{\epsilon_m}^2]$.

— $p(\mathbf{s}(t))$ or $p(\mathbf{s}(t)|\mathbf{z}(t))$: For this, first, in general, we assume that the sources are *a priori* independents, i.e., $p(\mathbf{s}(t)) = \prod_j p(s_j(t))$ or only conditionally independent, i.e. $p(\mathbf{s}(t)|\mathbf{z}(t)) = \prod_j p(s_j(t)|z_j(t))$. Then, we have either to choose expressions for $p(s_j(t))$ such as GG or for $p(s_j(t)|z_j(t))$, for example in the case of MoG.

— For the Markovian models, in general, we choose a first order Markov chain in 1D case and a Markov field with first order neighborhood in 2D case (images). For example, in 1D signals

$$p(s_j(0)) = N(0, \sigma_j^2), \quad p(s_j(t)|s_j(t-1)) = N(s_j(t-1), \sigma_j^2)$$

and for images where $t \in \mathcal{T}$ represents a pixel position and $t' \in \mathcal{V}(t)$ the neighboring pixels positions

$$p(s_j(t)|s_j(t'), t' \in \mathcal{T}_{-t}) \propto \exp \left[-\alpha_j \sum_{t' \in \mathcal{V}(t)} \phi(s_j(t), s_j(t')) \right]$$

where ϕ is the potential associated to the cliques of the Markov field neighborhood system.

— For the Markovian models for the discrete valued hidden variables $q_j(t)$ and $z_j(t)$, we use the Ising and Potts models respectively. For example

$$p(z_j(0) = k) = \pi_{jk}, \quad p(z_j(t) = k | z_j(t-1) = l) = \pi_{jkl}$$

and for images

$$p(z_j(t)|z_j(t'), t' \in \mathcal{T}_{-t}) \propto \exp \left[-\alpha_j \sum_{t' \in \mathcal{V}(t)} \delta(z_j(t) - z_j(t')) \right]$$

where $\delta(t) = 1$ for $t = 0$ and $\delta(t) = 0$ for $t \neq 0$.

— Finally, we also have to assign prior laws to the elements of the matrix \mathbf{A} and to the hyperparameters Θ such as the noise covariance \mathbf{R}_ϵ or only the noise variances $\theta_\epsilon = \{\sigma_{\epsilon_i}^2\}$, the parameters of the source distributions such as $\theta_s = \{(m_{jk}, \sigma_{jk}^2)\}$. In general, we choose conjugate priors for the hyperparameters.

When all these priors are appropriately assigned, we can obtain an expression for the posterior law

$$p(\mathbf{S}, \mathbf{Z}, \mathbf{A}, \Theta | \mathbf{X}) \propto p(\mathbf{X} | \mathbf{S}, \mathbf{A}, \theta_\epsilon) p(\mathbf{S} | \mathbf{Z}, \theta_s) p(\Theta) \quad (14)$$

where $\mathbf{S} = \{s(t), t \in \mathcal{T}\}$, $\mathbf{Z} = \{z(t), t \in \mathcal{T}\}$, $\mathbf{X} = \{x(t), t \in \mathcal{T}\}$ and $\Theta = \{\mathbf{A}, \theta_\epsilon, \theta_s\}$. We can then use this posterior law to define an estimator such as Joint Maximum A Posteriori (JMAP) or the Posterior Means (PM). The first needs optimization algorithms and the second integration methods. Both are computationally demanding. Alternate optimization is generally used for the first while the MCMC techniques are used for the second. We present here three such algorithms:

Algorithm A:	Algorithm B:	Algorithm C:
$\hat{\mathbf{S}} \sim p(\mathbf{S} \hat{\mathbf{Z}}, \hat{\mathbf{A}}, \hat{\Theta}, \mathbf{X})$	$\hat{\mathbf{S}} \sim p(\mathbf{S} \hat{\mathbf{Z}}, \hat{\mathbf{A}}, \hat{\Theta}, \mathbf{X})$	$\hat{\mathbf{S}} \sim p(\mathbf{S} \hat{\mathbf{Z}}, \hat{\mathbf{A}}, \hat{\Theta}, \mathbf{X})$
$\hat{\mathbf{Z}} \sim p(\mathbf{Z} \hat{\mathbf{S}}, \hat{\mathbf{A}}, \hat{\Theta}, \mathbf{X})$	$\hat{\mathbf{Z}} \sim p(\mathbf{Z} \hat{\mathbf{A}}, \hat{\Theta}, \mathbf{X})$	$\hat{\mathbf{Z}} \sim p(\mathbf{Z} \hat{\mathbf{A}}, \hat{\Theta}, \mathbf{X})$
$\hat{\mathbf{A}} \sim p(\mathbf{A} \hat{\mathbf{Z}}, \hat{\mathbf{S}}, \hat{\Theta}, \mathbf{X})$	$\hat{\mathbf{A}} \sim p(\mathbf{A} \hat{\mathbf{Z}}, \hat{\Theta}, \mathbf{X})$	$\hat{\mathbf{A}} \sim p(\mathbf{A} \hat{\Theta}, \mathbf{X})$
$\hat{\Theta} \sim p(\Theta \hat{\mathbf{A}}, \hat{\mathbf{S}}, \hat{\mathbf{Z}}, \mathbf{X})$	$\hat{\Theta} \sim p(\Theta \hat{\mathbf{A}}, \hat{\mathbf{Z}}, \mathbf{X})$	$\hat{\Theta} \sim p(\Theta \hat{\mathbf{A}}, \mathbf{X})$

In these algorithms, \sim represents either *argmax* or *generate sample using*. The first is used for alternate optimization and the second for MCMC Gibbs sampling. Implementing the **Algorithm A:** is easy, because, in general we have all the expressions of all the conditional laws used. The **Algorithm B:** needs integration with respect to the sources and **Algorithm C:** integration with respect to the sources and the hidden variables.

5 Examples of applications

The proposed methods have been used with success in different applications. Here we give references to some of these works:

Spectrometry: The model used is **Model 1** with *a priori* Gamma prior laws for both the sources and the mixing matrix elements. The estimator is the joint MAP and the implemented algorithm is alternate maximization with respect to sources, the mixing matrix elements and the hyperparameters (S. Moussaoui et al. [23, 24, 25]).

Source separation in astrophysics: One of the problems in astrophysics imaging is to separate different cosmic activities and in particular the Cosmological Microwave Background (CMB). The observation model, when written in Fourier domain is exactly as in (1), but here t represents the frequency. The example provided here is a simulation in the case where there are 3 sources and 6 observations. The appropriate model here **Model 3** and the implemented algorithm is an EM like [26, 27, 28, 29].

Source separation in satellite imaging: In the following references, two results in an application related to eliminating clouds in satellite imaging are presented. In the first example, the model used is **Model 4** where the pixels of each source image are assumed to be in one of the two classes [28]. The second example concerns the same problem but in wavelet domain where the same methods have been used when the separation is modeled in the wavelet domain. The main advantage being that simpler *a priori* models such as **Model 1** or **Model 2** can be used more efficiently. The following figure shows an example of

results obtained using either a Generalized Gaussian (GG) or a Mixture of two Gaussians (MoG) models [30, 31].

Data reduction, classification and segmentation of hyper-spectral images: Hyper-spectral images data are often represented as a set of images $x_{\omega}(\mathbf{r})$. However, a specificity of these images is that the pixels at a position \mathbf{r} along the wavelength bands ω form a spectral line. This is the reason for considering also these data as a set of spectra $x_{\mathbf{r}}(\omega)$. In both representations, the data are dependent in both spatial positions and in spectral bands. In [32, 33] the models **Model 5** or **Model 6** has been used to do jointly data reduction, classification and segmentation of hyper-spectral images.

6 Conclusion

The Bayesian estimation approach pushes farther the limits of classical PCA and ICA based methods for blind sources separation. In this work, we proposed six different models for the prior laws of the sources which can be used in different applications. The two first models are classical, the third accounts for temporal evolution of stationary sources. The fourth model which account for contours in images is appropriate for piecewise stationary sources, and finally, the fifth and sixth models are particularly appropriate for piecewise homogeneous sources. We then showed a few examples of simulation results which show different application areas of such models in spectrometry, in astrophysical imaging, in satellite and in hyperspectral imaging.

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