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ON-THE-FLY SPECTRAL UNMIXING FOR REAL-TIME HYPERSPECTRAL DATA ANALYSIS

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ABSTRACT

This paper presents an online linear unmixing method leveraging Kalman filtering for real-time analysis of hyperspectral data. Unlike traditional methods that require processing of the entire data set, the proposed approach sequentially updates pure spectra estimates as new data is acquired, that is, on a spectrum-by-spectrum basis, thereby significantly reducing computational cost. Experiments conducted on synthetic and real Raman data sets demonstrate that the proposed method achieves a favorable trade-off between unmixing accuracy and computational efficiency, making it suitable for real-time hyperspectral imaging applications.

Index Terms— multivariate curve resolution, pure spectra extraction, online processing, Kalman filter

1. INTRODUCTION

Hyperspectral (HS) imaging is a technology used for sample analysis with applications in various fields [1, 2, 3]. Although HS sensors have good spectral resolution, they suffer from limited spatial resolution, leading to the measurement of mixed spectra and making their interpretation challenging. Under a linear mixing assumption, the observations can be modeled as follows

$$D = CS^T + E, \quad (1)$$

where $D \in \mathbb{R}_+^{N \times L}$ contains N observations of spectral dimension L . Matrices $S \in \mathbb{R}_+^{L \times K}$, $C \in \mathbb{R}_+^{N \times K}$, and $E \in \mathbb{R}^{N \times L}$ represent the pure spectra, concentrations and error term, respectively, with K denoting the number of pure spectra. For analysis purposes, we seek to estimate S and C from the measured spectra D . This problem, termed spectral unmixing (SU) or multivariate curve resolution, has been tackled in several ways.

A well-known method addressing the SU problem is the multivariate curve resolution (MCR-ALS)[4]. MCR-ALS estimates S and C via alternating minimization, fixing one variable at a time and solving the resulting problem until convergence. In addition to enforcing positivity on these variables, other constraints can be incorporated, such as unimodality, closure, among others.

Alternative SU approaches have been proposed in the remote sensing literature, including geometric methods. Under the sum-to-one (closure) constraint, observations lie within a simplex whose vertices are the PS. This has led to a class of geometric methods which assume the presence of pure spectra among the data. Known methods making this assumption are vertex component analysis (VCA) [5] and N-finder (N-FINDER) [6]. However, this assumption is often violated in real-world scenarios, leading to alternative methods such as simplex identification via split augmented Lagrangian (SISAL) [7] and minimum volume simplex analysis (MVSA) [8], which seek to identify the smallest simplex enclosing the observations.

The effectiveness of SU methods is closely tied to the quality of data acquisition. However, obtaining high-quality data can be challenging, as it often requires significant time and may expose biological samples to harmful high-power laser. Recent innovations [9, 10] have aimed to overcome these hurdles by focusing on essential spectral pixels (ESs), which represent the most distinct spectral components. The authors in [9] proposed a Fourier domain approach to identify ESs, which has proven to be well-suited for online processing.

SU methods typically operate in an offline mode, requiring access to the full data set, which is impractical for real-time applications such as in situ monitoring or fast-paced biological imaging. To fill this gap, this paper aims at deriving an online SU algorithm able to operate on-the-fly. On-the-fly SU can be interpreted as an online source separation problem. Existing methods for achieving this task include online dictionary learning (DL) [11] and variants [12, 13]. These algorithms update the basis matrix (analogous to PS in SU) as

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new data are collected. However, they do not incorporate dimensionality reduction, which raises complexity issues when dealing with HS data. Additionally, experiments indicate that the online DL scheme proposed in [11] underperforms in the context of online SU due to a suboptimal update rule.

This paper proposes an online SU method based on the Kalman filter (KF) [14]. This method, referred to as KF-OSU, addresses the aforementioned limitations of traditional SU approaches by allowing dynamic updates of pure spectra (PS) estimates. Exploiting the concept of ES, the proposed method incorporates Fourier-based dimension reduction to enhance computational efficiency, making it well suited for real-time applications.

2. PROPOSED METHOD

This work assumes that the number K of PS is known a priori. In addition, the mixing concentrations are assumed to be subject to a sum-to-one constraint. It removes the scaling ambiguity [15] and allows interpreting concentrations as proportions. Note that this assumption is not very restrictive in the sense that it can be imposed via a normalization of the data.

2.1. The online mixing model

In an online context, one wants to update the pure spectra estimates as a new spectrum is acquired without reprocessing all measured spectra so far. To achieve this, we introduce a stochastic process of the form $\mathbf{S}_n = f_n(\mathbf{S}_{n-1})$ to model the evolution of the estimates, where n indexes the sequence of observations. This approach enables the update of the PS estimates, leveraging the information from the newly acquired spectrum \mathbf{d}_n and the current estimates $\hat{\mathbf{S}}_{n-1}$, without need of reprocessing all previous observations. We therefore introduce the following online mixing model:

$$\mathbf{d}_n = \mathbf{S}_n \mathbf{c}_n + \mathbf{e}_n, \quad (2)$$

$$\mathbf{S}_n = \mathbf{S}_{n-1} + \mathbf{V}_n, \quad (3)$$

where $\mathbf{e}_n \sim \mathcal{N}(\mathbf{0}, \sigma_e^2 \mathbf{I}_L)$ represents the observation noise, \mathbf{I}_L the identity matrix of size L and $(\mathbf{V}_n)_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma_v^2)$ is the process noise. Eq. (3) implies that the expectation of the PS at time index n is equal to the one at $n - 1$, which is a natural assumption.

The PS update can then be tackled within a Bayesian framework by deriving the conditional probability density function of \mathbf{S}_n given the observations up to time index n , i.e., $\mathbf{D}_{\leq n} = [\mathbf{d}_1, \dots, \mathbf{d}_n]$.

2.2. Online estimation of pure spectra

The concentrations are assumed to be known in this paragraph; their estimation will be discussed later. After vectorizing the online mixing model, using the vec operator which

stacks the columns of a matrix, the observation (2) and process (3) models write

$$\mathbf{s}_n = \mathbf{s}_{n-1} + \mathbf{v}_n, \quad (4)$$

$$\mathbf{d}_n = \mathbf{G}_n \mathbf{s}_n + \mathbf{e}_n, \quad (5)$$

with $\text{vec}(\mathbf{D}_n \mathbf{c}_n) = (\mathbf{c}_n^\top \otimes \mathbf{I}_L) \text{vec}(\mathbf{D}_n) = \mathbf{G}_n \mathbf{d}_n$, where \otimes is the Kronecker product operator. The sought posterior distribution is

$$p(\mathbf{s}_n | \mathbf{D}_{\leq n}) \propto p(\mathbf{d}_n | \mathbf{s}_n) p(\mathbf{s}_n | \mathbf{D}_{\leq n-1}),$$

which is Gaussian, thus fully defined by its mean and covariance matrix, which can be recursively computed through the KF as described in Algo. 1. The minimum mean square estimate of the PS is then defined as the mean of this Gaussian distribution.

The canonical form of KF imposes no constraint on the estimates, as can be seen in Algo. 1. In the SU context, the PS are expected to satisfy a positivity constraint, which can be easily achieved by setting all negative values to 0. However, Algo. 1 requires a matrix inversion of size proportional to the spectral dimension. This may not be computationally suitable for real-time processing due to the high spectral dimension. We thus introduce a dimension reduction step, discussed in the next section.

Algorithm 1: KF

Input : Newly measured spectrum \mathbf{d}_n , posterior mean $\boldsymbol{\mu}_{n-1}$ and covariance matrix $\boldsymbol{\Sigma}_{n-1}$ at time instant $(n - 1)$, observation matrix \mathbf{G}_n , uncertainty level σ_v^2 , model noise variance σ_e^2

// Predict the prior covariance matrix, compute the error

1 $\boldsymbol{\Sigma}_{n-1/2} \leftarrow \boldsymbol{\Sigma}_{n-1} + \sigma_v^2 \mathbf{I}_{KL}$

2 $\mathbf{r}_n \leftarrow \mathbf{d}_n - \mathbf{G}_n \boldsymbol{\mu}_{n-1}$

// Compute the innovation covariance and optimal gain

3 $\mathbf{Z}_n \leftarrow \mathbf{G}_n \boldsymbol{\Sigma}_{n-1/2} \mathbf{G}_n^\top + \sigma_e^2 \mathbf{I}_L$

4 $\mathbf{K}_n \leftarrow \boldsymbol{\Sigma}_{n-1/2} \mathbf{G}_n^\top \mathbf{Z}_n^{-1}$

// Update the posterior mean and covariance matrix

5 $\boldsymbol{\mu}_n \leftarrow \boldsymbol{\mu}_{n-1} + \mathbf{K}_n \mathbf{r}_n$

6 $\boldsymbol{\Sigma}_n \leftarrow (\mathbf{I}_L - \mathbf{K}_n \mathbf{G}_n) \boldsymbol{\Sigma}_{n-1/2}$

Output: Posterior mean $\boldsymbol{\mu}_n$ and covariance matrix $\boldsymbol{\Sigma}_n$ at time instant n .

2.3. Constrained PS estimation in a low-dimensional subspace

To alleviate the computational burden, we perform a dimensionality reduction via the Discrete Fourier Transform (DFT). The reduced version of each spectrum \mathbf{d}_n is computed as follows

$$\tilde{\mathbf{d}}_n = [\text{Re}(\mathbf{F}^\top \mathbf{d}_n) \text{Im}(\mathbf{F}^\top \mathbf{d}_n)]^\top, \quad (6)$$

where $\mathbf{F} \in \mathbb{C}^{L \times M}$ ($M \ll L$) contains M columns of the DFT matrix chosen so that $\mathbb{E} \left[\left\| \tilde{\mathbf{d}}_n \right\|_2^2 \right] \geq \alpha \mathbb{E} \left[\left\| \mathbf{d}_n \right\|_2^2 \right]$ for some $\alpha \in (0, 1]$. Thanks to the linearity of the DFT, the models introduced in (4) and (5) are still valid, and so is the PS update through Algo. 1. However, as the KF operates in the lower-dimensional subspace, we need to constrain the PS estimates $\hat{\mathbf{S}}_n$ such that their representation in the original subspace are nonnegative. We formulate this task as a regression problem, whose derivation is explained in what follows.

As observations $\tilde{\mathbf{d}}_1, \dots, \tilde{\mathbf{d}}_n$ are acquired, KF updates the estimate of the PS. This, produces a sequence of estimates $\hat{\mathbf{S}}_1, \dots, \hat{\mathbf{S}}_n$. Referring to the online mixing model, we have $\tilde{\mathbf{d}}_i \approx \hat{\mathbf{S}}_n \mathbf{c}_i$ for $i = 1, \dots, n$. Conversely, we can express $\hat{\mathbf{S}}_n$ as a linear combination of the spectra ($\tilde{\mathbf{d}}_i$). That is, we can find a regression matrix $\mathbf{R}_n \in \mathbb{R}^{P \times K}$ such that $\hat{\mathbf{S}}_n \approx \tilde{\mathbf{D}}_{1:P} \mathbf{R}_n$, where $\tilde{\mathbf{D}}_{1:P}$ contains some P spectra selected among the spectra ($\tilde{\mathbf{d}}_i$). Owing to linearity of the DFT, we can enforce the positivity constraint by solving the following regression problem

$$\min_{\mathbf{R}_n} \left\| \tilde{\mathbf{D}}_{1:P} \mathbf{R}_n - \hat{\mathbf{S}}_n \right\|_{\text{F}}^2 \quad \text{s. t.} \quad \mathbf{D}_{1:P} \mathbf{R}_n \geq \mathbf{0}. \quad (7)$$

In this way, the constrained PS estimates is $\hat{\mathbf{S}}_n^{(+)} = \mathbf{D}_{1:P} \hat{\mathbf{R}}_n$, where $\hat{\mathbf{R}}_n$ is the solution to (7).

2.4. Concentration estimation

When a new spectrum \mathbf{d}_n is acquired, it is necessary to determine the associated concentration \mathbf{c}_n to apply the KF. Drawing inspiration from the literature on online dictionary learning [11, 12, 13], we estimate \mathbf{c}_n by solving the following problem

$$\min_{\mathbf{c}} \left\| \mathbf{d}_n - \hat{\mathbf{S}}_n^{(+)} \mathbf{c} \right\|_2^2 \quad \text{s. t.} \quad \mathbf{c} \geq \mathbf{0}, \quad \mathbf{c}^\top \mathbf{1} = 1 \quad (8)$$

In this study, the problem defined by (8) is solved using the Sparse Unmixing by Variable Splitting and Augmented Lagrangian (SUnSAL) method [16].

2.5. The proposed online SU algorithm

The proposed algorithm is outlined in Algo. 2. For simplicity of presentation, the symbols for estimates have been omitted. The initial constrained PS estimate $\mathbf{S}_p^{(+)}$ can be obtained using any offline unmixing method applied to the first P observations.

3. EXPERIMENTS

We evaluate the proposed method on synthetic and real Raman data sets. We compare our method against three baseline

Algorithm 2: KF-OSU

Input : K (PS count), P (regressors count), spectra $\mathbf{D}_{1:P}$, noise variances σ_e^2, σ_v^2 , \mathbf{F} , initial PS estimate $\mathbf{S}_p^{(+)}$

- 1 $n \leftarrow P$
// Perform dimensionality reduction (see (6))
- 2 $\tilde{\mathbf{S}}_n^{(+)} \leftarrow \left[\text{Im}(\mathbf{F}^\top \mathbf{S}_n^{(+)}) \text{Im}(\mathbf{F}^\top \mathbf{S}_n^{(+)}) \right]^\top$
- 3 $\tilde{\boldsymbol{\mu}}_n \leftarrow \text{vec} \left(\tilde{\mathbf{S}}_n^{(+)} \right)$
- 4 $\boldsymbol{\Sigma}_n \leftarrow \sigma_v^2 \mathbf{I}_{2KM}$
- 5 **repeat**
- 6 $n \leftarrow n + 1$
// Estimate concentration \mathbf{c}_n and observation matrix \mathbf{G}_n
- 7 $\mathbf{c}_n \leftarrow \text{SUnSAL} \left(\mathbf{d}_n, \mathbf{S}_{n-1}^{(+)} \right)$
- 8 $\mathbf{G}_n \leftarrow \mathbf{c}_n^\top \otimes \mathbf{I}_{2M}$
// Perform dimensionality reduction (see (6))
- 9 $\tilde{\mathbf{d}}_n \leftarrow \left[\text{Im}(\mathbf{F}^\top \mathbf{d}_n) \text{Im}(\mathbf{F}^\top \mathbf{d}_n) \right]^\top$
// Update the posterior distribution
- 10 $(\tilde{\boldsymbol{\mu}}_n, \boldsymbol{\Sigma}_n) \leftarrow \text{KF} \left(\tilde{\mathbf{d}}_n, \tilde{\boldsymbol{\mu}}_{n-1}, \boldsymbol{\Sigma}_{n-1}, \mathbf{G}_n, \sigma_v^2, \sigma_e^2 \right)$
- 11 $\tilde{\mathbf{S}}_n \leftarrow \text{unvec}(\tilde{\boldsymbol{\mu}}_n)$
// Estimate the regression matrix by solving (7)
- 12 $\mathbf{R}_n \leftarrow \text{solve_regression} \left(\mathbf{D}_{1:P}, \tilde{\mathbf{D}}_{1:P}, \tilde{\mathbf{S}}_n \right)$
// Compute the constrained PS estimate in the original space and perform dimensionality reduction
- 13 $\mathbf{S}_n^{(+)} \leftarrow \mathbf{D}_{1:P} \mathbf{R}_n$
- 14 $\tilde{\mathbf{S}}_n^{(+)} \leftarrow \left[\text{Im}(\mathbf{F}^\top \mathbf{S}_n^{(+)}) \text{Im}(\mathbf{F}^\top \mathbf{S}_n^{(+)}) \right]^\top$
// Update the posterior mean
- 15 $\tilde{\boldsymbol{\mu}}_n \leftarrow \text{vec} \left(\tilde{\mathbf{S}}_n^{(+)} \right)$
- 16 **until** end of acquisition;

Output: Estimated PS matrix $\mathbf{S}_n^{(+)}$.

algorithms: MCR-ALS, VCA, and SISAL. These methods are used in an online setting by running them on the entire acquired spectra when a new one is measured. We first discuss the algorithm ability to estimate PS, then, their running time.

3.1. Data sets overview

Synthetic data sets: 220 data sets (5000 spectra each) were generated according to the model (1) with 4 spectra. Mixture concentrations were sampled from a Dirichlet distribution with parameter (1, 1, 1, 1), and spectra with over 70% of one primary spectrum were discarded. White Gaussian noise was added to achieve a 30dB signal-to-noise ratio (SNR).

Real data set: A 60×60×253 Raman image of an oil-in-water emulsion was acquired using a modified Instruments SA Explorer. Excitation was conducted at 633nm using a 20mW

HeNe laser, delivering around 5mW of power to the sample (for further details, refer to [17]). After unfolding, a 3600×253 matrix was obtained, along with 219 copies constructed by permuting the rows (i.e., the order of the acquired spectra).

3.2. Evaluation metrics

The performance of each method is assessed using the average spectral angle distance (aSAD), the root-mean-square error (RMSE), and the reconstruction error (RE) defined as $\text{aSAD} = \frac{1}{K} \sum_{k=1}^K \arccos\left(\frac{\hat{\mathbf{s}}_k^T \mathbf{s}_k}{\|\hat{\mathbf{s}}_k\|_2 \|\mathbf{s}_k\|_2}\right)$, $\text{RMSE} = \sqrt{\frac{1}{KN} \left\| \mathbf{C} - \hat{\mathbf{C}} \right\|_F^2}$, and $\text{RE} = \frac{\|\mathbf{Y} - \hat{\mathbf{C}} \hat{\mathbf{S}}^T\|_F}{\|\mathbf{Y}\|_F}$, respectively. The matrix $\hat{\mathbf{S}} = [\hat{\mathbf{s}}_1, \dots, \hat{\mathbf{s}}_k]$ (resp. $\hat{\mathbf{C}}$) contains the estimated PS (resp. concentrations). These metrics assess PS estimate accuracy and overall unmixing performance.

3.3. Results and discussion

Fig. 1 shows that VCA underperforms due to the absence of PS in the data, whereas KF-OSU, despite exhibiting slightly worse performance compared to MCR-ALS and SISAL, achieves low aSAD and RMSE values. This slightly worse lower performance can be attributed to the SNR, which affects KF-OSU more significantly than MCR-ALS and SISAL. Indeed, KF-OSU updates the PS based solely on the most recent observation, whereas MCR-ALS and SISAL leverage all acquired spectra, which explains their higher accuracy.

In the real data analysis (Fig. 2), all methods show low RE value, indicating a good spectra reconstruction and robustness to acquisition order.

We now discuss the runtime comparison. The experiments were conducted on a laptop with an Intel Core i7-8565U CPU (1.80GHz) and 8GB of RAM. The results demonstrate that KF-OSU is computationally efficient, requiring an average of 0.006 seconds per update for synthetic data sets and 0.005 seconds for real data set. In contrast, MCR-ALS, VCA, and SISAL were all slower. For the synthetic data sets, MCR-ALS took 1.9 seconds, VCA 0.06 seconds, and SISAL 0.17 seconds per update. For the real data set, MCR-ALS took 0.33 seconds, while VCA and SISAL required 0.04 and 0.1 seconds, respectively.

4. CONCLUSION

This paper introduces an on-the-fly spectral unmixing method that leverages Kalman filtering for real-time pure spectra extraction. The method is shown to be computationally efficient while demonstrating good performance in terms of pure spectra estimation, making it suitable for applications where real-time processing is required. Future developments could involve extending the proposed approach to handle nonlinear mixing models. A direction to tackle it could be to linearize the model and or to use variants of the Kalman filter, e.g.,

the extended Kalman filter, the unscented Kalman filter, the ensemble Kalman filter.

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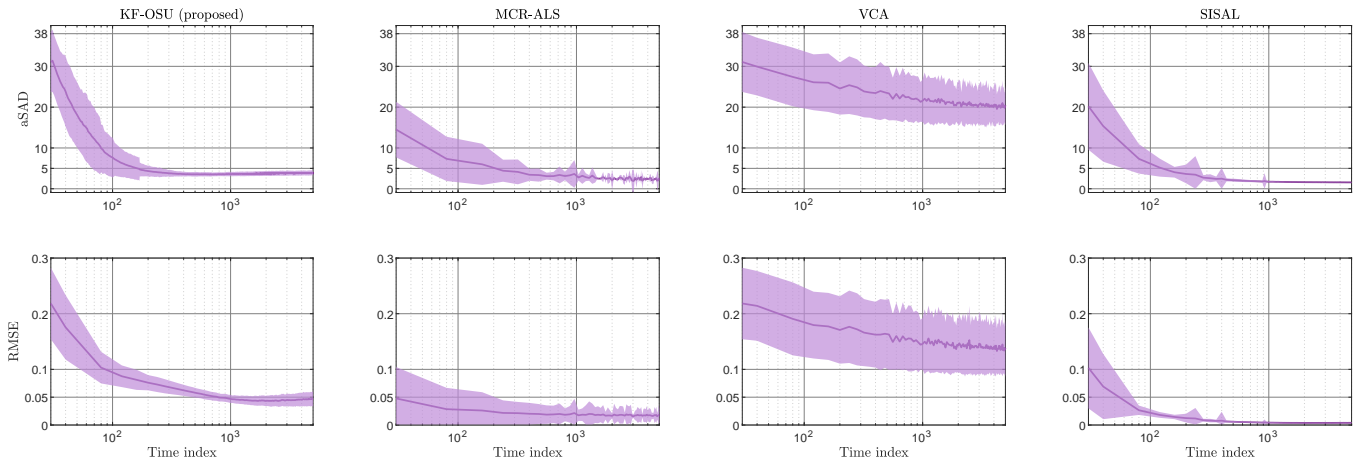


Fig. 1: Synthetic data sets: aSAD (top) and RMSE (bottom) vs. time index. Results averaged over 220 data sets; shaded areas indicate one standard deviation.

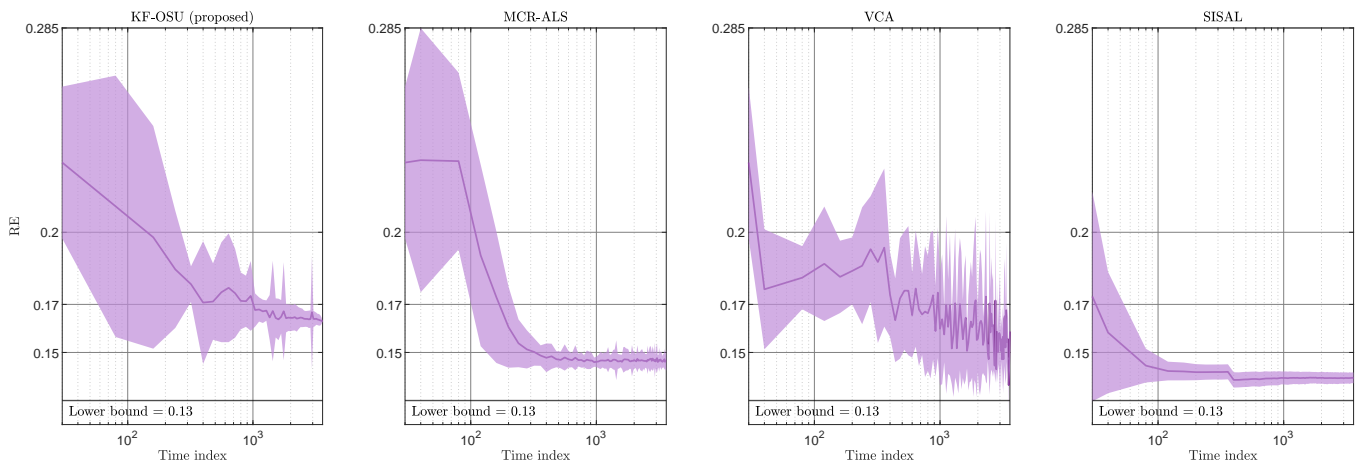


Fig. 2: Real data set: RE vs. time index. Results averaged over 220 data sets; shaded areas indicate one standard deviation. The lower bound corresponds to the minimum RE, estimated via principal component analysis. The number of pure spectra was set to 5.

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