A Unified Model of Feature Extraction and Clustering for Spike Sorting

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Abstract—Spike sorting plays an irreplaceable role in understanding brain codes. Traditional spike sorting technologies perform feature extraction and clustering separately after spikes are well detected. However, it may often cause many additional processes and further lead to low-accurate and/or unstable results especially when there are noises and/or overlapping spikes in datasets. To address these issues, in this paper, we proposed a unified optimisation model integrating feature extraction and clustering for spike sorting. Interestingly, instead of the widely used combination strategies, i.e., performing the principal component analysis (PCA) for spike feature extraction and K-means (KM) for clustering in sequence, we unified PCA and KM into one optimisation model, which reduces additional processes with fewer iteration times. Subsequently, by embedding the K-means++ strategy for initialising and a comparison updating rule in the solving process, the proposed model can well handle the noises and/or overlapping interference. Finally, taking the best of the clustering validity indices into the proposed model, we derive an automatic spike sorting method. Plenty of experimental processes and further lead to low-accurate and/or unstable results especially when there are noises and/or overlapping spikes in datasets. To address these issues, in this paper, we proposed a unified optimisation model integrating feature extraction and clustering for spike sorting. Interestingly, instead of the widely used combination strategies, i.e., performing the principal component analysis (PCA) for spike feature extraction and K-means (KM) for clustering in sequence, we unified PCA and KM into one optimisation model, which reduces additional processes with fewer iteration times. Subsequently, by embedding the K-means++ strategy for initialising and a comparison updating rule in the solving process, the proposed model can well handle the noises and/or overlapping interference. Finally, taking the best of the clustering validity indices into the proposed model, we derive an automatic spike sorting method. Plenty of experimental datasets confirm that our proposed method outperforms the related state-of-the-art approaches.

Index Terms—spike sorting, PCA, K-means, unified optimisation

I. INTRODUCTION

In the neuroscience community, extracellular recording, especially on the single-electrode and the extended tetrodes, remains the only way to provide single action potential resolution to understand the brain codes of large animals or human objects [1], [2], [3], [4]. Different neurons generate action potentials with a unique extracellular waveform (i.e., “spike”) [1], [5]. With these unique waveforms, assigning each spike to its tentative neuron becomes possible, and such procedure is called spike sorting [6], [7]. Outputs from spike sorting are beneficial in broad scopes of applications like neural prosthetic [8], brain-machine interfaces [9], treating epilepsy [6], etc. In real scenarios, since the recorded signals from extracellular implementations consist of mixture local field potentials, noises, spikes, etc., conventional spike sorting techniques firstly have to filter the signals to remove most unwanted noises and disturbances, leaving the filtered trace for the spike detection [5]. Afterwards, feature extraction and clustering on the detected spikes are needed, which are rather challenging compared with filtering and detection [10].

Over the past decades, numerous studies have been devoted to extracting discriminative spike features and clustering the featured spikes. On one hand, the spike feature extraction methods can be fallen into two categories: global-features-based and local-features-based ones. Global-features-based methods include principal components analysis (PCA) [11], Fourier transform [12], wavelet decomposition [13], [14], etc. Local-features-based methods are those called locality preserving projection (LPP) [13], Laplacian eigenmaps (LE) [15], and graph-Laplacian (GL) [17], etc. On the other hand, clustering methods are flourishing, e.g., K-means (KM) [16], [18], spectral clustering (SC) [15], [19], Gaussian mixture model (GMM) [20], [18]. Simply combining spike feature extraction and clustering, i.e., separately performing them in sequence, has achieved certain degrees of success.

However, it is unpractical to exhaust all kinds of potential combinations, and what’s worse, these combinations may yield unsatisfactory and unstable results for different datasets, especially when there are noises and/or overlapping spikes interference. For instance, suppose we have two noise-disrupted datasets obtained from global-features-based and local-features-based methods as shown in Fig.1a and Fig.1d respectively. For the global-featured spikes in Fig.1a, we yield a satisfactory result with KM method (Fig.1b), but an unsatisfactory result with SC (Fig.1c). Inversely, for the local-featured spikes in Fig.1d, opposite conclusions are drawn, i.e., the result of SC is satisfactory (Fig.1f) while that of KM method is not (Fig.1e).

Such problems are originated from at least the following three reasons: 1) the internal relationships between feature extraction and clustering methods are not considered when we simply combine them for spike sorting; 2) The features directly extracted from the detected spikes are sensitive to the noise interference from noises and/or overlapping spikes, without

1 Note that, for both KM and SC, different initial values will result in different outputs and we only show one of them randomly.
As the number of neurons increases, the result quality improves. By doing this, we can choose the number of clusters more flexibly. Therefore, both methods still suffer from unstable results.

Considering the feedback from the clustering stage, and unsupervised clustering methods themselves are sensitive to initial values, and may fall into local optimum, etc.

Recently, Keshtkaran et al. [21], [18] introduced linear discriminant analysis guided by K-means (LDAKM) [22], which tried to joint LDA with KM into a coherent framework, model the feature extraction and clustering problem in spike sorting. Subsequently, they take an additional GMM process after each KM iteration, proposing LDAGMM [19] to detect the overlapping spikes. Unfortunately, LDAKM confuses the matrix ratio trace together with trace ratio criteria in the framework, resulting in the outputs vibration or even mis-convergence [23], [24]. LDAGMM forces more different algorithms to be spliced together compared with LDAKM, which may distract the jointed model. Along with this distraction, more iteration times and computation resources are required. Therefore, both methods still suffer from unstable results.

Inspired by these efforts [21], [18], in this paper, we propose a unified optimisation model of feature extraction and clustering for spike sorting, intrinsically integrating PCA and KM, which enforces these two stages to pursue an identical criteria. In particular, by engaging alternating direction method [25], we alternatively update the extracted features and clustering results, which means the feedback from the clustering is considered in the feature extraction stage. Further, embedding K-means++ initialising and comparison updating strategies in the cluster step, the unstable problem is alleviated significantly. Finally, we derive an automatic spike sorting framework after estimating the number of neurons through existing validity indices. Our contributions are mainly three-fold:

- We theoretically give the solution to our proposed unified model, and also prove that it can be converted into the PCA or KM like process for each alternate updating. Besides, we provide its computational complexity analysis.
- We conduct various experiments on both synthetic and real-world datasets, which verify the monotonicity of our model, rather than vibration. The efficacy and stability of our proposed method are also confirmed.

The rest of this paper is organised as follows. In section II, our automatic spike sorting framework is given in details. Particularly, the newly unified feature extraction and clustering model and its solution are formulated and explained together with corresponding theoretical analysis, etc. Section III presents and discusses our experimental results. Finally, we conclude this paper in Section IV.

II. METHODS

In this section, the proposed automatic spike sorting framework is demonstrated in details. It includes filtering, spike detection, and the proposed unified feature extraction and clustering model integrating PCA with KM.

Filtering and amplitude threshold detection in [14] and [26] are engaged in our framework. Note that, the particular parameters in these two steps for different datasets are, by default, assigned according to [14], [26], and we will point out these default settings in Section II as well. Thereafter, each detected spike is stored in the matrix $X \in \mathbb{R}^{d \times n}$ in the form of a column. Here, $d$ and $n$ stand for the number of variables (dimensions) and the number of observations (spikes), respectively.

A. Theoretically Represent and Optimise PCA and KM

For easy representation, we first theoretically represent and optimise PCA and KM.

1) PCA: Given a detected spike dataset $X$, the target of PCA is to construct an orthogonal linear projection matrix $W \in \mathbb{R}^{d \times m}$ so that the projected spikes lie in the $m$ linear spaces with greatest data variances. Here, $m$ is the reduced dimension. The centralisation matrix is firstly formed by [24],

$$H = I - \frac{1}{n}N \in \mathbb{R}^{n \times n},$$

where $I$ and $N$ are, respectively, the identity matrix and the all-ones matrix, in which every element is 1. It can be checked that, $H$ is a symmetric and idempotent matrix [27], i.e., $H = H^T = HH^T$. Then, the spikes can be centred by rightly multiplying $H$, i.e., $XH$. PCA resorts to the total scatter matrix, $XH(XH)^T = XHX^T$, as,

$$\max_W \; W^TXHX^TW; \quad \text{s.t.,} \quad W^TW = I.$$ 

The above problem can be solved by performing eigenvalue decomposition (EVD) [27] on $XHX^T$. That is $XHX^T = \Lambda AW^{-1}$, where $\Lambda$ is the diagonal matrix whose diagonal entries are the corresponding eigenvalues and/or overlapping spikes exist or not.

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Fig. 1: (a) and (d) are featured spikes mapped on two dimensions which are supposed to be obtained from global-based and local-based feature extraction methods, respectively. (b) and (e) show the results from K-means while (c) and (f) from spectral clustering. For the spikes distributed in (a), K-means performs better than spectral clustering, while for (d) the conclusion is opposite.

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of $XHX^T$. Finally, we can get the optimal value and the optimum solution, $W^*$, with the biggest $m$ eigenvalues in $\Lambda$ and the corresponding $m$ eigenvectors in $W$, respectively.

2) KM: In KM, a label indicator matrix, $G = \{G_{ij}|i=1,...,n, j=1,...,c\} \in \mathbb{R}^{n \times c}$, is constructed by the rule that $G_{ij} = 1$ if the $i$-th spike belongs to the $j$-th class and other elements of $G$ are 0, where $c$ is the number of classes (i.e., neurons). Meanwhile, the centres of $c$ classes are stored as columns in the matrix $M \in \mathbb{R}^{d \times c}$. Then the entire KM clustering process can be expressed as searching for one appropriate local optima solution by performing expectation maximisation (EM) algorithm on the following problem \cite{28, 29}.

$$\min_{G,M} \|XH - MG^TG\|^2_F,$$

s.t., $G1_c = 1_n, G^T1_n > 1_c$, $G_{ij} \in \{0,1\}$,

where $\|X\|^2_F = \left(\sum_{i=1}^d \sum_{j=1}^n |X_{ij}|^2\right)^{\frac{1}{2}}$ is the Frobenius norm with respect to matrix $X$, $1_c \in \mathbb{R}^{1 \times c}$ is an all-ones column vector whose elements are 1, and $X \succ Y$ indicates $X_{ij} > Y_{ij}$ with element-wise inequality.

Theorem II.1. Let $X \in \mathbb{R}^{d \times n}$ be the input detected spikes, $\text{tr}(\cdot)$ be the trace operation, and $H \in \mathbb{R}^{n \times n}$ be centralisation matrix, i.e., $H = I - \frac{1}{n}1_n1_n^T$. Then Problem \cite{3} is equivalent to the following one.

$$\min_{G} \text{tr} \left( XH(I - G(G^TG)^{-1}G^T)HX^T \right),$$

s.t., $G1_c = 1_n, G^T1_n > 1_c$, $G_{ij} \in \{0,1\}$.

Proof. \cite{11} Denote $f(G,M) = \|XH - MG^TG\|^2_F$. Since $\|X\|^2_F = \text{tr}(XX^T) = \text{tr}(X^TX)$, we have,

$$f(G,M) = \text{tr} \left( XHX^T - 2MG^THX^T + MG^TG^TMG^T \right).$$

According to $\frac{\partial f(G,M)}{\partial M} = 0$ along with $\frac{\partial f}{\partial X} = \frac{\partial \text{tr}(XX^T)}{\partial X} = X + Y$, we can further derive,

$$M = XHG \left( G^TG \right)^{-1}.$$  \hspace{1cm} (4)

Combining Problem \cite{3} and Eq. \cite{4}, we get the result. \hfill \Box

Theorem II.1 indicates that KM can potentially be simplified from the core EM mechanism with iteratively updating two variables to the problem with only one variable needed to be solved.

B. Unify PCA and KM for Spike Feature Extraction and Clustering

In the conventional spike sorting procedure, KM is performed after doing PCA on the centralised data matrix, $XH$, for dimension reduction. That is to say, $W^T X H$ is actually fed into KM. In addition, PCA is a maximisation problem for pursuing the single variable, $W$, and KM has the potential to be transformed into a minimisation problem for pursuing the single-variable, $G$. By employing Theorem II.1 and a trace operation on the ratio of matrix \cite{30}, we can integrate PCA and KM into one optimisation problem as follows\cite{32}.

$$\max_{G,W} \text{tr} \left\{ W^T XH X^T W \right\},$$

s.t., $G1_c = 1_n, G^T1_n > 1_c$, $G_{ij} \in \{0,1\}$,

$$W^TW = I.$$

We engage the alternating direction method \cite{25} with two-updating steps to solve the above problem, which guarantees to converge.

1) Update $G$: When updating $G$, we ignore the constraint associated with $W$ and convert the maximisation problem to a minimisation one. Then Problem \cite{5} is converted to,

$$\min_{G} \text{tr} \left\{ W^T XH(I - G(G^TG)^{-1}G^T)HX^T W \right\},$$

s.t., $G1_c = 1_n, G^T1_n > 1_c$, $G_{ij} \in \{0,1\}$.

According to Theorem II.1 solving the above problem equals to performing the following KM-like procedure,

$$\min_{G} \left\| (W^T XH X^T W)^{-\frac{1}{2}} W^T XH - MG^T \right\|^2_F,$$

s.t., $G1_c = 1_n, G^T1_n > 1_c$, $G_{ij} \in \{0,1\}$,

where $M = (W^T XH X^T W)^{-\frac{1}{2}} W^T XHG (G^TG)^{-1}$. To get a better optimum, we use two strategies as follows,

- Different from randomly initialising the class centres, we make use of the well-known K-means++ \cite{31} initialisation strategy.

- To ameliorate the local optimum problem, we employ a comparison updating rule \cite{27} detailed as follows.

Updating Rule: We begin by defining that,

$$g(G,M) = \left\| (W^T XH X^T W)^{-\frac{1}{2}} W^T XH - MG^T \right\|^2_F.$$

Suppose that we obtain the solutions to Problem \cite{3}, $W^*_t$ and $G^*_t$ along with the corresponding $M^*_t$, after the $t$-th iteration. Before updating $G$ at the $(t+1)$-th iteration, we firstly initialise $\{M^*_t, M^*_t, ..., M^*_t\}$ by using K-means++ strategy, and calculate the corresponding $\{G^*_t, G^*_t, ..., G^*_t\}$. Here, $a$ denotes the number of initialisations, which is fixed to be 10 in our model. Then we update $G$ with the following criteria,

$$G^*_{t+1} = \begin{cases} G^*_t, & \text{if } g(G^*_t, M^*_t) < g(G^*_t, M^*_t); \\ G^*_t, & \text{otherwise}, \end{cases}$$

where $i = 1, 2, ..., a$, and $G^*_t$ is defined as the solution to following problem,

$$\min_{G} \left\| \left( W^*_t^T XH X^T W^*_t \right)^{-\frac{1}{2}} W^*_t^T XH - M^*_t G^T \right\|^2_F,$$

s.t., $G1_c = 1_n, G^T1_n > 1_c$, $G_{ij} \in \{0,1\}$.\footnote{Generally speaking, there are, at least, four ways, including ratio trace, ratio determinant, trace linear combination and trace ratio, to integrate PCA and KM into one objection criteria as shown in \cite{32}. But in this paper, we only focus on the trace ratio in view of its convenience for optimising and presenting, etc.}
Algorithm 1 The algorithm for solving Problem (5)

Input: The detected spikes \( X \in \mathbb{R}^{d \times n} \), the number of neurons \( c \).

Output: Transformation matrix \( W^* \in \mathbb{R}^{d \times m} \), the allocation results of spikes \( G^* \in \mathbb{R}^{n \times c} \).

1: Initialise \( m = c - 1 \), \( t = 1 \); Define \( H \in \mathbb{R}^{n \times n} \), \( W(0) \in \mathbb{R}^{d \times m} \), and \( G(0) \in \mathbb{R}^{n \times c} \) according to Eqs. (1), (2), and (3), respectively.
2: Update \( W_t \) according to Proposition 1.
3: Update \( G_t \) according to Eq. (8).
4: Quit the loop if \( G_t = G_{t-1} \), otherwise, \( t = t + 1 \) and go back to step 2.
5: Return \( G^* = G_t \) and \( W^* = W_t \).

Algorithm 2 Proposed automatic spike sorting procedure

Input: The recorded spike signal; The initial reduced dimension \( m_0 \).

Output: Transformation matrix \( W^* \in \mathbb{R}^{d \times m} \), the allocation results of spikes \( G^* \in \mathbb{R}^{n \times c} \), and the estimated number of neurons \( \tilde{c} \).

1: Filter and detect the recorded signal to get the spikes signal matrix \( X \in \mathbb{R}^{d \times n} \). Start initially reduced dimension, only affects the estimation of the number of neurons after the model initialisation and before the main iterative optimisation.
2: Automatically Estimating the Number of Neurons: Although many spike sorting methods determine the number of neurons by manually specifying or graphically merging and decomposing clusters [17, 26, 52], integrating existing estimation methods into the model can reduce a lot of unnecessary human intervention [21]. To this end, we integrate the estimation of the number of neurons after the model initialisation and before the main iterative optimisation. New within a range of the number of neurons in initial settings, the spike sorting algorithm is pre-run to obtain a series of corresponding index values, and then one reasonable number of neurons is picked up based on the best index value [12]. [34]. Two clustering validity indices, Calinski Harabasz [34] and gap [15], are employed in this paper.
3: Automatically Determining the Number of Features: To efficiently reduce the time consumption and further free human intervention, in our method, automatically determining the dimensions of spikes is adopted. Specifically, \( m_0 \), as the initially reduced dimensions, only affects the estimation of the number of neurons. After estimating the number of neurons \( \tilde{c} \), \( m = \tilde{c} - 1 \) is recommended, where \( m \) denotes the dimension of the spike in iteration process. This strategy not only reduces computational complexity in each iteration but avoids the singularity problem [23] in EVD.

Finally, our proposed automatic spike sorting procedure is summarised in Alg. 2.

III. EXPERIMENTS

The proposed automatic spike sorting method is evaluated on both several well-known simulated datasets and the real tetrode-recorded dataset. Further, we compared it with several related state-of-the-art spike sorting methods on different evaluation criteria, including neurons estimation, accuracy, time consumption, stability, etc. All codes of our experiments are implemented in MATLAB R2020a, which is run on a personal computer with Intel Core i7-8750H 2.20 GHz CPU, 32G RAM.)
A. Experimental Datasets and Evaluation Criteria

Four challenging synthetic neural datasets in Wave_clus [14], [35], which own the ground truths, are used in our simulations. They are Easy1_noise*, Easy2_noise*, Difficult1_noise*, and Difficult2_noise*, in which the asterisk stands for the embedded noise standard deviation (i.e., noise level) with respect to the main waveforms. Here, the waveforms were issued by three neurons in neocortex and basal ganglia [35], and the noise was mimicked by randomly selecting the real recorded signal with different amplitudes from different neurons [14]. Note that, ‘Easy’ reflects that the used waveforms are easy to distinguish (i.e., they are different from each other) and vice versa for the ‘Difficult’. Besides, the noise level of ‘Easy1’ is ranging from 0.05 to 0.4 with the step length 0.05 while those of the rest three datasets are in [0.05, 0.2].

We also engaged the publicly available vivo dataset, HC1 [3] in our real-world experiment. HC1 was recorded from the anesthetized rat hippocampus using an extracellular tetrode, with which one extra intracellular electrode was implanted to a single neuron to obtain its actual spike times (refer to ground truth) for evaluation [30], [36].

To take the best detected spike in simulation datasets and avoid errors from detection, we pick up spikes based on the ground truth for Wave_clus. Then, with the detected spike matrix X, we evaluated the performance of determining the number of neurons, clustering accuracy, time consumption, etc. Especially, to reflect the stability, we conducted 20 independent trials, which resulted in corresponding means and their standard deviations. As for the real-world dataset, HC1, the F1 related criteria, false negative rate (FNR, or called as Miss rate) and false positive rate (FPR), are used. Here, the false negative represents that the predicted cluster is negative but the real class is true, while the false positive means the predicted cluster is positive but the real class is false. FNR and FPR are reasonable enough to reflect the clustering results, and lower values for both of them mean better performances [26], [18].

B. Experiments on Synthetic Dataset - “Wave_clus”

Same as the original works [14], [35], “Wave_clus” was filtered with passband located at 300 – 6,000 Hz firstly. But different from the default configuration using amplitude thresholds to detect spikes, we directly extracted those spikes by using a 64 sample-length window from the known spike time in ground truths. This facilitates to get consistent spike datasets to perform fair comparison with different methods.

1) Determination of the Number of Neurons: Four automatic spike sorting methods (LE-KM [16], LPP-SCK [15], LDAKM [21], LDAGMM [18], and the Wave_clus [14] baseline, respectively. P1 and P2 refer to our proposed model with Calinski Harabasz and gap index for estimating the number of neurons.

### Table I: The number of estimated neurons using various automatic spike sorting methods on Wave_clus datasets with (without) overlapping spikes.

| DS           | NL       | With Overlapping Spikes (Without) |
|--------------|----------|----------------------------------|
|              | A        | B                                | C        | D        | E        | P1       | P2       |
| Easy1 05    | 2(3)     | 2(10)                            | 2(4)     | 3(2)     | 3(3)     | 3(5)     |          |
| 10           | 3(3)     | 6(9)                             | 2(4)     | 2(5)     | 3(3)     | 3(3)     |          |
| 15           | 8(2)     | 2(4)                             | 3(2)     | 2(4)     | 3(3)     | 3(3)     |          |
| 20           | 3(2)     | 2(7)                             | 2(5)     | 3(5)     | 3(3)     | 3(3)     |          |
| 25           | 2(7)     | 2(2)                             | 2(3)     | 2(4)     | 6(3)     | 3(3)     |          |
| 30           | 3(2)     | 8(3)                             | 2(5)     | 2(5)     | 3(3)     | 3(3)     |          |
| 35           | 3(3)     | 4(2)                             | 4(5)     | 4(3)     | 3(3)     | 3(3)     |          |
| 40           | 4(3)     | 2(2)                             | 2(4)     | 4(3)     | 3(3)     | 3(3)     |          |
| Difficult1 05 | 6(7)   | 6(10)                            | 2(4)     | 2(4)     | 2(4)     | 3(6)     | 6(6)     |
| 10           | 3(2)     | 2(3)                             | 2(4)     | 2(6)     | 3(3)     | 3(3)     |          |
| 15           | 2(2)     | 2(6)                             | 2(6)     | 3(2)     | 3(3)     | 2(2)     |          |
| 20           | 4(3)     | 2(2)                             | 2(5)     | 3(7)     | 4(3)     | 3(3)     |          |
| Difficult2 05 | 8(3)   | 3(8)                             | 2(4)     | 2(3)     | 4(3)     | 3(3)     |          |
| 10           | 9(3)     | 3(6)                             | 2(5)     | 2(4)     | 3(3)     | 2(3)     |          |
| 15           | 9(3)     | 2(10)                            | 2(3)     | 2(3)     | 4(2)     | 2(2)     |          |
| 20           | 8(4)     | 2(9)                             | 3(4)     | 2(4)     | 3(3)     | 2(2)     |          |
| Total Hit    | 8(7)     | 4(3)                             | 2(6)     | 2(5)     | 13       | 14(15)   | 16(13)   |

DS and NL are the names and the noise levels of datasets, respectively. A, B, C, D, and E stand for the automatic spike sorting frameworks of LE-KM [16], LPP-SCK [15], LDAKM [21], LDAGMM [18], and the Wave_clus [14] baseline, respectively. P1 and P2 refer to our proposed model with Calinski Harabasz and gap index for estimating the number of neurons.
dataset without the influence from overlapping spikes. It can be seen from Table I that the results of our proposed method reach the baseline level and relatively outperform those of LE-KM, LPP-SCK, LDAGMM, and LDAKM. The main reasons include, 1) the estimation results from LE-KM and LPP-SCK are sensitive to the reduced dimensions of features. 2) For LDAGMM and LDAKM, the estimation process is mixed in the iteration optimisation, making the results susceptible to the model’s random initial point and vibrant iteration. 3) Our proposed method integrated with Calinski Harabasz or gap index succeed largely with the stable input of the estimation from PCA initialisation as shown in Eq. (2).

2) Overall Accuracy and Time Consumption: Secondly, the overall accuracy and time consumption of various spike sorting methods are compared. The state-of-the-art spike feature extraction methods, PCA [11], LE [16], LPP [15], GF [17], LDA [21], [18], along with three automatic spike sorting schemes, LE-KM [16], LPP-SCK [15], LDAGMM [21], [18] are compared. Noted that the results of LDAGMM, which are similar to those of LDAKM, are not shown here due to the space limitation. Further, we also compared either PCA or GF with KM and SCK as spike sorting methods for more general comparisons. For the sake of fair comparison, the number of neurons and the reduced dimension for each method are assigned as 3 and 2, respectively.

Specifically, in LE-KM, the number of nearest neighbours is, by default, set to be 12, however, the number of times to randomly repeat KM is not specified, and we set it to be 10 (it is equal to the number of K-means++ initialisations in our proposed method as mentioned in subsection II-B1). Besides, the points of landmarks in SCK and the number of neighbours for each sample in LPP are, by default, fixed to be 1000 and 5, respectively. As for LDAKM, the open-source code is publicly accessed [40], while the configurations of our proposed method are detailed in Alg.I. Note that, 20 independent times are performed in each method on each dataset and the final average results along with its standard deviation are recorded. In our experiments, whether the overlapping spikes exist or not in the datasets is compared.

As shown in Table II without overlapping spikes, nearly all methods could get acceptable results on datasets with small noise levels. But when the noise level increases, it seems that only the model-based method (i.e., LDAKM and our proposed method) can maintain high accuracy, while other combined feature extraction and clustering in sequence methods failed. On the other hand, the results of methods combined with SCK (i.e., PCA-SCK, LPP-SCK, GF-SCK) and LDAGMM are not stable. For example, the standard deviations of the average accuracy for LDAKM are around 5% and those for the SCK-based methods are even more than 15% in the datasets of Easy2_noise05, Difficult1_noise10, etc. The standard deviations of the methods combined with KM (i.e., PCA-KM, LE-KM, GF-KM) are comparable with setting a sufficient number of initialisation, however, the average accuracies are not satisfactory. On the contrary, by initialising with K-means++ strategy and updating with comparison rule whose details are shown in section II-B1 our proposed method obtains the near-perfect accuracies. At the same time, the processing time is also less than others. What’s more interesting is that by calculating the standard deviation of the processing time, the minimum processing time of our proposed method is equal to the simple combined method, PCA-KM. This means the proposed method can automatically adjust the processing time according to the complexity of the dataset. These findings

3 Please visit the link, https://github.com/HLBayes/Unified-SS to access the Matlab codes about the proposed method in this paper.
are also consistent with the presence of overlapping spikes as shown in Table III in which the exact processing time of our method on each dataset is manifested.

3) Monotonicity Experiments: Finally, in order to verify the monotonicity of our proposed method, we graph the model objective value versus the times of iteration. The results on Difficult1-noise5 and Difficult1-noise20 are illustrated while other datasets with similar results are ignored. At the same time, we also compared the model-based spike sorting methods, LDAKM and LDAGMM. As shown in Fig.5, the proposed method always iterates towards the increasing objective values and converges after about 10 iterations. Although LDAKM has a trend of increasing the objective values overall, its optimal value is not always increasing, since the objective function of the two-step solution for LDAKM is different [24]. Furthermore, LDAGMM adds GMM operations after each KM [18], making its objective value even iterate toward a decreasing direction. LDAKM and LDAGMM need more iterations (Fig.5a and Fig.5b), and also more computational resources (Tables I and III).

C. Experiment on Real-world Dataset - “HCl”

In this section, the real-world dataset, HCl [8], is used and four automatic spike sorting methods, LE-KM [16], LPP-SCK [15], LDAKM [21], LDAGMM [18], are compared. Similar as [26, 18], we firstly filter the raw recorded signal using a highpass Butterworth filter at 250 Hz with order 50. Then, spikes were identified by exceeding a threshold that is assigned by [26]. For more detailed preprocessing about the spike filtering and detection, please refer to the open source [41]. Actually, after these preprocessings, all the ground truth spikes recorded by the intracellular electrode are detected. Then the spikes from the tetrode are concatenated into a vector for further automatic sorting. Finally, according to the existing ground truth intracellularly recorded from one neuron, we can obtain the corresponding FPR and FNR.

In Figure 4 the results of five automatic spike sorting methods are shown when the estimated neurons ranges from 2 to 5. Among them, the actual estimated results are emphasised with bold dots and their numerical values are also accompanied. On one hand, it is easy to find that the results of LDAKM, LPP-SCK, and LDAGMM are unstable, especially the standard deviation of the FNR of LPP-SCK reaches 39.2%. On the other hand, LDAKM and our proposed method get better results for different estimated neurons compared with LE-KM, LPP-SCK and LDAGMM, although the average estimated number is different between them (the proposed method is 3 while LDAKM is 5).

In addition to FPR and FNR, we also showed the mean waveforms of ground truth and the distribution of spikes obtained by different methods. Specifically, assuming the estimated number of neurons is $\hat{c}$, when $\hat{c} \leq 3$, the graphical dimension is $\hat{c} - 1$ while when $\hat{c} > 3$, the dimension is 3. Meanwhile, the average waveform from each class of spike is also shown under the corresponding panel. As we can see from Fig.5, the number of neurons and their waveforms obtained by various methods are different. Relatively speaking, the results of our proposed method are better since the graphical results show three distinctly different clusters and waveforms. In contrast, the results of LE-KM (Fig.5a) and LPP-LCK (Fig.5c) do not separate the spikes reasonably. With further analysing the average waveforms, we can see that the second (red) waveforms from our proposed method are more consistent with the ground truth compared with the third (yellow) waveforms from LDAKM and the second (red) waveforms from LDAGMM. Besides, it appears that the
Fig. 3: The optimal value versus the times of iteration on two datasets of (a) LDAKM, (b) LDAGMM, and (c) our proposed method.

Fig. 4: FPR and FNR obtained by several automatic spike sorting methods, i.e., LE-KM, LDAKM, LPP-SCK, LDAGMM and our proposed one on the HCI1 datasets. Here, results with the estimated neurons from 2 to 5 are included, and among them, the bold dots indicate the actual estimated results (along with their standard deviation) for each method.

first (blue) and second (red), fourth (purple) and fifth (green) waveforms of LDAKM (Fig. 5d) are very similar, and we prefer to merge them together. Similarly, for LDAGMM (Fig. 5e), the third (yellow) and fourth (purple) waveforms are also very similar.

In summary, our proposed method exhibits excellent accuracy and stability in both synthetic and real-world datasets.

IV. CONCLUSIONS

This paper studied a optimisation problem for spike sorting which unified the feature extraction and clustering. It was basically solved in an integrated framework with PCA and K-means. The computational complexity of this model is linear to the number of spikes, which is less than existing methods. In particular, we proposed an efficient and effective automatic spike sorting method after integrating existing strategies to estimate the number of neurons. The yielded satisfactory and stable results on both synthetic and real datasets verified the efficacy of our proposed method.

APPENDIX A

PROOFS

Proof (of Proposition 1): Let $S_1 = XHX^T$ and $S_2 = XHX(I - G(G^TG)^{-1}G^T)HX^T$, we can simplify (10) as,

$$\max_W\{\mathrm{tr}\left(W^T S_1 W\right)\},$$

s.t., $W^TW = I$.

Because $S_1$ and $S_2$ are symmetric matrix, there exists a $d \times d$ nonsingular square matrix $A$ so that,

$$A^T W^T S_2 W A = I_d,$$

and $A^T W^T S_1 W A = M_d$, (A.2)

where $M_d$ is a $d \times d$ diagonalised matrix. According to (B.3), (B.4), (A.1), and (A.2), we have,

$$S_2^{-1} S_1 W = W \left(W^T S_2 W\right)^{-1} \left(W^T S_1 W\right) = W \left(A^T \right)^{-1} I_d A^{-1} \left(A^T \right)^{-1} M_d A^{-1} = W A M_d A^{-1},$$

that is, $S_2^{-1} S_1 W A = W A M_d$. Besides,

$$\mathrm{tr}\left(W^T S_1 W\right) \approx \mathrm{tr}\left(W^T S_2 W\right) \approx \mathrm{tr}\left(A^T W^T S_2 W A\right) = \mathrm{tr}\left(A^T W^T S_1 W A\right).$$

Therefore, the optimal value of (A.1) can be determined by the $m$ largest eigenvalues of $M_d$. Also the corresponding eigenvectors in $WA$ are the optimal solution of (A.1). Certainly such eigenvalues and eigenvectors could be deduced from generalised eigenvalue decomposition on $S_2^{-1} S_1$, so they also satisfy the decomposition (11) and Proposition 1 is proved.
Fig. 5: The mean waveform of ground truth is shown in (a), along with the low-dimensional distributions of spikes and their mean waveforms of each cluster from several automatic spike sorting schemes: (b) LE-KM, (c) LPP-LCK, (d) LDAKM, (e) LDAGMM, and (f) our proposed method.

APPENDIX B
MAIN MATHEMATICAL PROPERTIES

The following equations are used in the Appendix A

\[
\frac{d}{dX} \text{tr} \left\{ X^T Y X \right\} = (Y + Y^T) X
\]

\[\text{(B.1)}\]

\[
\frac{d}{dX} \text{tr} \left\{ Y X^T S X \right\} = -S X (X^T S)^{-1} (Y + Y^T) (X^T S)^{-1}
\]

\[\text{(B.2)}\]

\[
\frac{d}{dX} \text{tr} \left\{ \frac{X^T S_1 X}{X^T S_2 X} \right\} = \frac{d}{dX_1} \text{tr} \left\{ \frac{X^T S_1 X}{X^T S_2 X} \right\} \bigg|_{X_1=X} + \frac{d}{dX_2} \text{tr} \left\{ \frac{X^T S_1 X}{X^T S_2 X} \right\} \bigg|_{X_2=X} = -2S_2 X (X^T S_2 X)^{-1} (X^T S_1 X) (X^T S_2 X)^{-1} + 2S_1 X (X^T S_2 X)^{-1}
\]

\[\text{(B.3)}\]

When (B.3) is set to be equal to zero, we have

\[
S_2^{-1} S_1 X = X \left( X^T S_2 X \right)^{-1} (X^T S_1 X).
\]

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