I-SEA: Importance Sampling and Expected Alignment-based Deep Distance Metric Learning for Time Series Analysis and Embedding

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Abstract

Learning effective embeddings for potentially irregularly sampled time-series, evolving at different timescales, is fundamental for machine learning tasks such as classification and clustering. Task-dependent embeddings rely on similarities between data samples to learn effective geometries. However, many popular time-series similarity measures are not valid distance metrics, and as a result they do not reliably capture the intricate relationships between the multi-variate time-series data samples for learning effective embeddings. One of the primary ways to formulate an accurate distance metric is by forming distance estimates via Monte-Carlo-based expectation evaluations. However, the high-dimensionality of the underlying distribution, and the inability to sample from it, pose significant challenges. To this end, we develop an Importance Sampling based distance metric – I-SEA – which enjoys the properties of a metric while consistently achieving superior performance for machine learning tasks such as classification and representation learning. I-SEA leverages Importance Sampling and Non-parametric Density Estimation to adaptively estimate distances, enabling implicit estimation from the underlying high-dimensional distribution, resulting in improved accuracy and reduced variance. We theoretically establish the properties of I-SEA and demonstrate its capabilities via experimental evaluations on real-world healthcare datasets.

1 Introduction

Learning to embed time-series is at the heart of a number of machine learning tasks such as classification (Hayashi, Mizuhara, and Suematsu 2005), clustering (Ma et al. 2019), forecasting (Murray 1993), recommendation, search and retrieval (McFee, Barrington, and Lanckriet 2012) (Oord, Dieleman, and Schrauwen 2013). Furthermore, representations which encode the geometry of the data are also fundamental for other data mining and information retrieval tasks with applications in healthcare (Yang and Shahabi 2004) (Xiong and Chen 2006), speech processing (Sakoe and Chiba 1978), music retrieval (McFee, Barrington, and Lanckriet 2012) (Oord, Dieleman, and Schrauwen 2013), and human activity understanding (Tran and Sorokin 2008) (Jiang, Jr, and Gonzalez 2012), meteorology and climate (Lhermitte et al. 2011), Baranowski et al. 2015).

Measuring distances between data samples is key for faithfully encoding the geometries for embedding. To this end, time-series are compared based on their similarity under a certain monotonic and non-decreasing arrangement, or alignment (Sakoe and Chiba 1978). Notwithstanding their success, popular methods rely on an optimal alignment, which prevents them from constituting a valid distance metric (Müller 2007) (Mei et al. 2015) (Cuturi and Blondel 2017), an essential property for reliably capturing the geometry via pair-wise distances (Cover and Hart 1967) (Cox and Cox 2008).

Moreover, time-series metric learning, which learns supervised task-dependent embeddings via linear or non-linear (deep learning-based) transformations to capture complex temporal relationships among the features in multi-variate time-series (Xing et al. 2002) (Salakhutdinov and Hinton 2007), Weinberger and Saul 2009 (Hoffer and Ailon 2015), also critically relies on effective pair-wise distance comparisons to learn embeddings such that the distances in the transformed space reflect the nearest neighbor properties imposed by the supervision (Shalev-Shwartz, Singer, and Ng 2004). However, since popular ways to compare time-series do not constitute a distance metric, the learned representations or embeddings based on such measures also do not encode the complex relationships between the data samples (Cover and Hart 1967) (Cox and Cox 2008). This situation is further exacerbated by irregular sampling, missing entries and other non-idealities. As a result, developing reliable distance metrics for time-series remains a challenging problem.

One way to form a valid distance metric is by averaging distances over all possible alignment paths (Cuturi et al. 2007) (Che et al. 2017). However, these averages (Expected Alignments) are difficult to compute accurately since the computations involve expectation evaluations w.r.t a high-dimensional distribution over all alignment paths. This problem is further compounded by a) the inability to sample from this distribution due to the combinatorial nature of the problem (even when known), and b) the distribution being over rare events (since good alignments are rare).

To address these challenges, we propose I-SEA: Importance Sampling and Expected Alignment-based distance metric for comparing time-series, which leverages a) deep learning-based representations to capture complex temporal
feature dependencies, and b) Non-parametric Density Estimation and Weighted Importance Sampling for accurate distance estimation, to learn effective embeddings of multi-variate time-series. Our specific contributions are as follows:

- **Importance Sampling-based data-driven distance metric for time-series.** We develop a deep learning and Importance Sampling-based distance metric which learns a task-dependent metric using a large margin-based triplet loss metric learning approach. We establish the theoretical properties of I-SEA, showing that it is a valid distance metric for comparing time-series.

- **Improved distance estimation via Importance Sampling.** Adopting a rare event distribution view of the similarity distribution over alignment paths, we develop a Weighted Importance Sampling-based approach, which utilizes Adaptive Non-parametric Density Estimation and Rejection Sampling to enable implicit estimation from an inherently high-dimensional distribution. The resulting metrics are accurate and exhibit reduced variance properties across different datasets.

- **Learning faithful embeddings.** Our neural network-based representations and distance estimation effectively encode the relationships between time-series. Furthermore, our estimation procedure shows low variance, while conventional Importance Sampling estimators are known to result in high variance if the distribution over desired region has a small support (Precup 2000).

A key contribution of our work is to enable accurate distance computations by implicit estimation from a distribution over all alignment paths using Importance Sampling. The primary challenge here, in addition to the high-dimension of the distribution, is that as opposed to conventional Importance Sampling, sampling over time-series involves two distributions – one over the alignment path lengths, and other over all alignment paths of a specific length. Although both are a priori unknown, our main result leverages the fundamental differences between these two to develop Importance Sampling-based metrics for time-series. As a result, our contributions here provide, to the best of our knowledge, the first task-dependent metric using a large margin-based triplet loss metric learning approach. We establish the theoretical properties of I-SEA, showing that it is a valid distance metric for comparing time-series.

### 1.1 Related Works

**Comparing Time-series.** Classical similarity measures such as dynamic time warping (DTW) (Müller 2007) and multiple sequence alignment (MSA) (Hogeweg and Hesper 1984), rely on an alignment step before comparing the time-series, independent of the data. Global Alignment Kernel-based (GAK) methods also belong to this class although leverage the kernel-trick to compute alignment over all paths to develop a metric (Cuturi et al. 2007, Cuturi 2011). Application-specific measures are a popular way to compare time-series (Qiu et al. 2019), but these often do not constitute a metric. On the other hand, recent optimal transport-based metrics do not consider the sequence order (Huang et al. 2016). To mitigate this, Su and Hua (2018); Su and Wu (2019) develop a locally order-preserving variant of the Wasserstein metric. However, these works do not consider the intra-sequence relationships nor show if they constitute a valid metric; see also Shanmugam (2018).

**Deep Metric Learning.** Task-dependent metrics learn an embedding by transforming the data either linearly or non-linearly (Xing et al. 2002). These rely on alignment computations on the transformed data to develop a similarity measure. Since linear transformation-based methods (Laugier et al. 2014, Mei et al. 2015) fail to capture the complex dependencies across features in multivariate time-series metric learning, deep learning-based metric learning has gained popularity (Hoffer and Ailon 2015), leading to gradient training amenable loss function for end-to-end training (Cuturi and Blondel 2017), and alignment-independent techniques (Mueller and Thyagarajan 2016). As a result, metric learning inherently relies on faithfully computing pairwise distances to learn an embedding (Weinberger and Saul 2009).

**Importance Sampling and Rare Event Distributions.** Importance sampling is a Monte-Carlo variance reduction method, also used to estimate expectations w.r.t. a distribution while drawing samples from a different one (Precup 2000, Rubinstein and Kroese 2016). Since choosing a sampling distribution is critical for controlling the estimation error (specifically for rare event distributions), adaptive strategies leverage Monte-Carlo sampling to simultaneously estimate the sampling distribution and the target expectation for both parametric (Karamchetan, Björner, and Cornell 1989) and non-parametric (Zhang 1996) densities; see also Glynn and Iglehart (1989).

### 2 I-SEA: Methodology

I-SEA has two main components to address the two key challenges to develop a valid metric for multi-variate time-series: a) accurate distance computation between time-series, and b) capturing complex feature dependence structure using data-driven representations. We now detail each of these, with our overall metric learning-based architecture shown in Fig 1 and notations summarized below.\(^1\)

\(^1\)Notation: We denote vectors and matrices by bold lower x and capital X case letters, respectively. \(E[\cdot]\) denotes the expectation operator. \(\|\cdot\|\) denotes the 2-norm. \(U(t;\cdot)\) denotes the discrete uniform distribution. Let \(X \in \mathbb{R}^{n \times T_X}\) be a multi-variate time-series where \(n\) denotes the number of variables and \(T_X\) denotes the number of time steps. For a time-series \(X\), \(X_{\alpha_U} \in \mathbb{R}^{n \times U}\) denotes the arrangement of columns of \(X\) according to indices of an integer-valued vector \(\alpha_U \in \mathbb{R}^U\) (which can have repeated entries). We use \(X_{\alpha_U}(t) \in \mathbb{R}^n\)
2.1 Distance computations via Importance Sampling and Expected Alignment

Time-series evolving at different time scales are compared via a process called alignment (Sakoe and Chiba 1978). Alignment finds correspondences between two time-series by selecting the entries of one w.r.t. another in a monotonically non-decreasing fashion. Formally, an alignment path $A_U := (\alpha_U, \beta_U)$ for multi-variate time-series $X \in \mathbb{R}^{n \times T_X}$ and $Y \in \mathbb{R}^{n \times T_Y}$ is defined as follows.

**Definition 2.1.** An alignment path $A_U$ between two time-series is defined as a pair of monotonically non-decreasing sequences $(\alpha_U, \beta_U)$, where $\alpha_U, \beta_U \in \mathbb{U}^U$.

Here, the sequences $\alpha_U$ and $\beta_U$ denote the indices chosen from the time-series $X$ and $Y$, respectively. With this, the distance over an alignment path between two multi-variate time-series $X \in \mathbb{R}^{n \times T_X}$ and $Y \in \mathbb{R}^{n \times T_Y}$ for an alignment path $A_U := (\alpha_U, \beta_U)$ of length $U$ is formalized as follows.

**Definition 2.2.** For a distance metric $d(\cdot)$, the distance $D_{A_U}^{(X,Y)}$ between multivariate time-series $X \in \mathbb{R}^{n \times T_X}$ and $Y \in \mathbb{R}^{n \times T_Y}$ under the alignment path $A_U$ is defined as

$$D_{A_U}^{(X,Y)} = D_{\alpha_U, \beta_U} := \sum_{t=1}^{U} d(X_{\alpha_U}(t), Y_{\beta_U}(t)).$$

Here, we use the distance metric $d(\cdot)$ (say Euclidean distance) to compute the local distance between vectors $X_{\alpha_U}(t)$ and $Y_{\beta_U}(t)$ in $\mathbb{R}^{n}$ for a given alignment path $A_U$.

**Expectation w.r.t a High-dimensional Distribution.** Equipped with a metric over an alignment path, averaging across distances over alignment paths (Expected Alignment) leads to a valid distance metric (Cuturi et al. 2007; Cuturi 2011; Che et al. 2017), as opposed to that over a single path (Sakoe and Chiba 1978). Our crucial observation is that a naive averaging by considering all alignment paths to be of equal importance may not be accurate. In other words, two time-series may have higher similarity only along a few alignment paths, i.e. they may be rare. As a result, a naive averaging may lead to inaccurate estimates by being agnostic to the underlying similarity structure, as shown in Fig. 2(a).

**Importance Sampling.** Formally, let $p(\cdot)$ denote the distribution over all alignment paths $A_U$ of length $U$, where the distribution has higher weight for better alignment paths, shown in Fig. 2(b). It would indeed be ideal if we could sample from a distribution $p(\cdot)$ which reflects the similarity structure (or distances) over the alignment paths between the time-series. However, since these alignment paths and the corresponding distances are unknown a priori, (and $p(\cdot)$ is unknown, in general) we cannot sample directly from $p(\cdot)$.

We can, however, sample uniformly over all alignment paths, say a distribution $q(\cdot)$, and assess the goodness of a path $A_U$ after observing it, and use these scores to adjust the distance estimate. To this end, we leverage Importance Sampling (Precup 2000; Rubinstein and Kroese 2016) to evaluate the expectation w.r.t. $p(\cdot)$, while drawing samples using $q(\cdot)$.

**Significance.** I-SEA can leverage any type of Importance Sampling approach depending upon the application. We here present a Weighted Importance Sampling and adaptive Non-parametric Density Estimation-based approach specifically suited for the case when favorable alignments are rare. Our analysis can be of independent interest for Importance Sampling for time-series data. In our discussion, we use cosine similarity-based scores $s(A_U) \in [0,1]$ to assess an alignment path (shown below).

$$s(A_U) := \frac{(1+\cos \theta)}{2}$$

where $\cos \theta = \frac{\text{Tr}(Y_{\beta_U}^T X_{\alpha_U})}{\|X_{\alpha_U}\|_F \|Y_{\beta_U}\|_F}$. (2)

Cosine-similarity is a popular choice for computing pairwise similarity between matrices. It is independent of the
length of the time series since it focuses on the angle between two vectors (Schütze, Manning, and Raghavan [2008]). Based on the time-series, other choices may include linear, polynomial, sigmoid (and soft-max), Radial Basis Function (RBF), and Laplacian scoring functions (Zhang et al. [2007]).

Non-parametric Density Estimation and Weighted Importance Sampling. The primary challenge here is the high-dimensionality of \( p(\cdot) \), which is a distribution over all alignment paths between two multi-variate time-series. There are two sources of randomness here: the choice over \( a) \) the alignment path lengths \( U \), and \( b) \) all alignment paths of length \( U \), denoted by \( A_U \). To this end, we leverage Non-parametric Adaptive Kernel Density Estimation to estimate the distribution over alignment lengths \( U \sim f(U) \), and Weighted Importance Sampling strategy for the distribution over alignment paths. Overall, the I-SEA \( D_{I-SEA} \) is defined as follows.

**Definition 2.3.** For alignment path length \( U \sim f(U) \) supported on \( \{U_1, U_h\} \), and a corresponding alignment path \( A_U \sim p(A_U) \), for a distribution \( p(\cdot) \) over alignment paths \( A_U \) of length \( U \), the Importance Sampling and Expected Alignment-based distance metric, \( D_{I-SEA} \) is defined as

\[
D_{I-SEA}(X, Y) := \mathbb{E}_U \left[ \mathbb{E}_{A_U} \left[ D_{I-SEA}^{(X,Y)}(A_U) \right] \right] = \sum_{U \in \{U_1, U_h\}} f(U) \sum_{A_U \in A_U} D_{I-SEA}^{(X,Y)}(A_U) p(A_U),
\]

where \( D_{I-SEA}^{(X,Y)}(A_U) \) denotes the distance between \( X \) and \( Y \) under the alignment path \( A_U \) (Def. 2.2).

Next, Thm. 1 establishes the validity of \( D_{I-SEA} \) as a distance metric, as follows (proof in Supp. A.1).

**Theorem 1.** For a distance metric \( d(x, y) \) for \( x, y \in \mathbb{R}^n \), the distance \( D_{I-SEA}(X, Y) \) between two multi-variate time-series \( X \in \mathbb{R}^{n \times T_X} \) and \( Y \in \mathbb{R}^{n \times T_Y} \) defined in Eq. (3) is a valid distance metric. Namely, it satisfies the following:

1. Non-negativity: \( D_{I-SEA}(X, Y) \geq 0 \).
2. Symmetry: \( D_{I-SEA}(X, Y) = D_{I-SEA}(Y, X) \), and
3. Triangle Inequality: \( D_{I-SEA}(X, Z) \leq D_{I-SEA}(X, Y) + D_{I-SEA}(Y, Z) \).

**Estimating I-SEA.** Alg. 1 details the overall Importance Sampling-based procedure to form I-SEA for given time-series \( X \) and \( Y \). Although I-SEA yields a valid metric as per Thm. 1, the distributions \( f(\cdot) \) and \( p(\cdot) \) are both unknown \textit{a priori}. Our key observation is that there is a difference between the properties of these two distributions. Since \( f(\cdot) \) is a distribution over alignment lengths, it is a one-dimensional distribution and if were indeed known, we can sample from it using Monte Carlo sampling techniques. However, since \( p(\cdot) \) is a distribution over all alignment paths of a given length, it is potentially a very high-dimensional distribution, and even if it were known, we may not be able to sample from it directly. We leverage this difference to decouple these distributions to formulate our estimator as discussed below.

**Non-parametric Adaptive Density Estimation for \( f(\cdot) \).** We pose \( f(\cdot) \) estimation as a Non-parametric Density Estimation problem, that we accomplish via weighted Kernel Density Estimation (KDE) by adaptively improving the estimate using \( p(\cdot) \) as weights for each path with kernel \( \kappa(\cdot) \) (Zhang et al. [1996]). The number of adaptive steps \( k \) to update \( f(\cdot) \) can be chosen based on the computation budget. To sample path length \( U \) using the KDE estimate \( \hat{f}_k(\cdot) \) of \( f(\cdot) \), we use Rejection Sampling (Shapiro [2003]) at each step.

**Weighted Importance Sampling for \( p(\cdot) \).** We leverage Importance Sampling[4] that allows us to sample the alignment paths \( A_U \) according to a distribution \( q(\cdot) \) to form an Importance Sampling estimator \( \hat{D}_{I-SEA} \) of \( D_{I-SEA} \) w.r.t. the target distribution \( p(\cdot) \) using the estimator

\[
\hat{D}_{I-SEA} := \frac{1}{m} \sum_{i=1}^{m} D_{I-SEA}^{(X,Y)}(A_i) p(A_i) q(A_i),
\]

5: For each \( u \in \{U_1, U_h\} \), update \( \hat{f}_{k+1}(\cdot) \) using Weighted KDE from samples \( \{U_i\}_{i=1}^{m} \) with \( (p(A_i))_{i=1}^{m} \) as weights by \( \hat{f}_{k+1}(u) = \frac{1}{m+h} \sum_{i=1}^{m+h} p(A_i) \kappa \left( \frac{U_i - u}{h} \right) \).

This importance-based weighting is effective in forming an estimate where the important region is relatively small (Precup [2000]). For \( q(\cdot) \), we utilize an algorithm for uniformly sampling over the alignment paths presented in Alg. [B.1] in Supp. B. In general, \( q(\cdot) \) can be any tractable distribution. The estimate \( \hat{D}_{I-SEA} \) is indeed an unbiased estimator of \( D_{I-SEA} \) as established by the following lemma (proof in Supp. A.2).

**Lemma 2.** If the alignment paths are sampled as per a distribution \( q(\cdot) \), then for \( U \sim f(U) \) supported on \( \{U_1, U_h\} \), and \( A_U \sim q(\cdot) \), \( D_{I-SEA} \) can be estimated as

\[
D_{I-SEA}(X, Y) = \mathbb{E}_U \left[ \mathbb{E}_{A_U} \left[ D_{I-SEA}^{(X,Y)}(A_U) q(A_U) \right] \right].
\]

To mitigate the case where we only sample bad alignment paths, the following result establishes the number of samples
we observe that the procedure succeeds with lower number will encounter a similar dependence.

Time Complexity. For time-series of average length \( T \), and \( U_h = O(T) \), I-SEA requires \( O(T^2) \) samples (say \( c_1 T^2 \)) from Lem. 3 for some \( c_1 > 0 \). Let the distance computations for each path take \( O(T) \) time. Then the overall time complexity is \( O(T^3) \), which is similar to Che et al. [2017], and the constant number of KDE steps do not change the overall order. Note that the dependence on the length is a natural consequence of using concentration results used to establish sufficient conditions for the success of the estimation with high probability. As such, sampling based methods will encounter a similar dependence. Nevertheless in practice, we observe that the procedure succeeds with lower number of samples, the complexity can be controlled by restricting range of \( U \), which still results in a valid distance metric.

2.2 Deep Metric Learning

I-SEA leverages neural network to transform the multi-variate time-series before utilizing the Importance Sampling-based distance computations (described in the previous section). To accomplish this, we train a neural network to learn an appropriate non-linear transformation for effectively embedding of the multi-variate time-series data. To this end, we adopt a triplet loss-based large margin approach (Weinberger and Saul [2009]) for this exposition. Note that I-SEA can be trained with other deep metric learning loss functions; see [Kaya and Bilgel 2019]. These loss functions rely on computing pair-wise distances to learn an embedding that captures the relationship between data samples effectively (Weinberger and Saul [2009]). Since the triangle inequality holds for distance metrics, training via the metric learning loss learns an effective transformation, capturing the relative geometry (Cover and Hart [1967]; Shalev-Shwartz, Singer, and Ng [2004]; Cox and Cox [2008]; Weinberger and Saul [2009]). Specifically, the large margin approach aims to learn an embedding of the time-series data samples, by bringing a data sample \( X^{(i)} \) closer to its in-class targets (in the embedding space), while pushing away from the out-of-class imposters (using the triplet loss) (Weinberger and Saul [2009]; Che et al. [2017]). Formally, given \( N \) samples \( \{X^{(i)}\}_{i=1}^N \) from \( C \) classes, the targets \( S^+_i \), and the imposters \( S^-_i \) for the \( i \)-th data sample, we minimize the following objective by the choice of I-SEA’s neural-network parameters in \( D_{\text{I-SEA}}(\cdot) \),

\[
\min_{D} \sum_{i \in [N], j \in S^+_i} D^{(i,j)} + \lambda \sum_{i \in [N], j \in S^+_i, k \in S^-_i} \max\{\delta + D^{(i,j)} - D^{(i,k)}, 0\},
\]

where \( D^{(i,j)} := D(X^{(i)}, X^{(j)}) \) is the distance metric and \( \lambda \) denotes a non-linear transformation of \( X \) learned via a neural network \( f_{NN}(\cdot) \), i.e., \( \hat{X} = f_{NN}(X) \). Here, \( \lambda \) and \( \delta \) control the separation between classes (margin).

3 Experimental Evaluation

We evaluate and compare the performance of I-SEA for metric learning tasks arising in two real-world healthcare time-series datasets which suffer from one of more of the following non-idealities such as missing data, irregular sampling, and a large feature set. We now describe the experiments; see Supp. C for raw data embeddings (Fig. C.1), details of the set-up, additional results, and baselines descriptions. The code is available at https://github.com/srambhatla/ISEA
We evaluate the performance of I-SEA with popular datasets. We downsample these traces (by a factor of 4) resulting in data samples of length 32 “UCI-EEG (32)” and 64 “UCI-EEG (64)”, respectively, with a feature-set of 37 variables. The UCI EEG dataset (Goldberger et al. 2000) consists of in-hospital Intensive Care Unit (ICU) patient medical data recorded over the first 48 hours of their stay, and the eventual mortality outcome (0 or 1). We randomly sample 1108 traces to form a balanced dataset containing observations from 37 variables observed irregularly over the 48 hour period with missing entries (73%/sample), aggregating the observations for each hour. The resulting samples are of length 48 with a feature-set of 37 variables.

### 3.2 Variants and Baselines

We evaluate the performance of I-SEA with popular task-dependent and independent baselines for time series analysis. We present two variants of I-SEA in the experiments to study the contribution of a) Weighted Importance Sampling (WIS) and b) Gaussian Kernel-based (\(\kappa(\cdot)\)) KDE for estimating \(f(\cdot)\). Here, the first variant “I-SEA (WIS-Unif)” incorporates WIS only (i.e., \(f(\cdot)\) is set to be Uniform distribution) and is used to analyze performance with respect to Che et al. (2017) that does not use WIS; The second variant “I-SEA (WIS-KDE)” incorporates both WIS and KDE. We employ Euclidean distance for \(d(\cdot, \cdot)\), and fix the hyper-parameters across all experiments; see Supp. C. We use data independent measure such as Multi-variate DTW (MDTW), Multiple Sequence Alignment (MSA) (Hogue and Hesper 1984), Global Alignment Kernel (GAK) (Cuturi 2011), and task-dependent measures such as Decade (Che et al. 2017), neural network-based Soft-DTW (Cuturi and Blondel 2017), neural network-based MDTW (MDTW-NN), Manhattan Neural Network (Ma-NN) (Mueller and Thyagarajan 2016) and LDMLT (LogDet divergence based Metric Learning with Triplets) (Mei et al. 2015). Of these, Decade (when Euclidean distances are used to compute local distances), Ma-NN, MSA, and GAK constitute a metric. For task-dependent baselines, we use the large margin metric learning loss shown in Eq. 7. For the neural network-based baselines, we use a two-layer feed-forward model with sigmoid activations to capture complex feature dependence with the same input and output dimensions.

### 3.3 Evaluation Metrics

We use the K-Nearest Neighbor Mean Accuracy over the test sets corresponding to the 5 folds and its standard deviation to evaluate the embeddings learned using the techniques. Here, we evaluate the performance of the techniques for various values of \(K\), i.e. \(K \in \{1, 3, \ldots 19\}\). In addition, we evaluate the learned visualizations both qualitatively and quantitatively, via Multidimensional Scaling (MDS)-based 2-D projections (training) since MDS can handle metrics and non-metrics, and in terms of \(\text{triplet loss} - \%\text{ violation of triangle inequality over triplets} (20k \text{ random triplets each for train and test set}), \) respectively, using the learned distances.

### 3.4 Results

**K-Nearest Neighbor Performance.** We compare the performance of I-SEA with the baselines detailed in Supp. C.1 based on their K-Nearest Neighbor (K-NN) classification accuracy for metric learning tasks for the real-world datasets. Panels (a), (b), and (c) in Fig. 3 show the K-NN Misclassification (1- Accuracy) performance of the baselines as compared to I-SEA for UCI-EEG (32 and 64), and the PhysioNet dataset respectively; see Supp. C.2 for detailed results. We also show the corresponding distribution of standard deviation across \(K\)'s in the violin plots in panels (d), (e), and (f) of Fig. 3 respectively. We observe that across datasets, I-SEA variants perform better across different choices of \(K\).
while also exhibiting the best variance properties, i.e., both low and consistent. This is because Importance Sampling at its core is a variance reduction method and leads to superior variance properties across datasets. This underscores the benefit of Importance Sampling for computing the Expected Alignment. These also point to learned embedding properties. Specifically, even as the number of neighbors grow, the K-NN performance for I-SEA is stable, indicating that the learned metric faithfully separates the in-class and out-of-class examples. This can also be observed to some extent in Decade and Ma-NN, highlighting the importance of a valid metric for time-series deep metric learning.

Analyzing the Learned Embeddings. In Fig. 4 we visualize the learned distances by I-SEA and the baselines using the 2-dimensional MDS embedding based on the pair-wise training set distances (over the last training fold) for the UCI-EEG (32); see Supp. 1 (Figs. C.2 and C.3) for other datasets. Complementary to these results, we show the percent triplet violations (violations of triangle inequality by data triplets) by each method over train and test sets for these (for the same fold) in Fig. 5. The embeddings are revealing in terms of how distance computations are used by metric learning. Specifically, we notice that all deep metric learning techniques – which use the large margin approach shown in Eq. 4 – exhibit some kind of clustering structure, while the rest of the baselines do not, highlighting the role of deep learning for metric learning.

Next, we observe that the MDTW-NN baseline for both datasets shows a clustering which seems to lie on a line. This is because although deep representations do help with separation, the pair-wise similarities cannot capture relationships between data samples. This can also be observed from Fig. 5 where we analyze triplet violations over 20k randomly chosen triplets. Generally, metrics (I-SEA, Decade, Ma-NN, GAK, MSA) perform better than similarity measures (Soft-DTW, MDTW-NN, MDTW). Furthermore, among the neural network-based methods, valid metrics (I-SEA, Decade, Ma-NN) outperform the non-metrics (Soft-DTW, MDTW-NN). These underscore the importance of distance metrics for reliable time-series embedding.

Overall, our results demonstrate the importance of a) a valid distance metric, b) Importance Sampling-based method to tackle high-dimensional distributions, and c) deep metric learning to capture complex feature dependence for learning effective time-series embeddings.

4 Discussion

Summary. Data-driven task-dependent metrics are critical for learning effective time-series embeddings. These learning procedures rely on computing pair-wise similarities to effectively encode the geometrical relationships in the given data. However, unlike distance metrics, similarity measures do not reliably represent the relationships between data points from pair-wise measurements. In this work, we develop a data-driven metric for multi-variate time-series data – I-SEA – which estimates the distance between data samples using Expected Alignment. A key contribution here is to enable accurate Expected Alignment computation by developing a way to implicitly estimate the expectation w.r.t. a (high-dimension) distribution over all alignment paths using Non-parametric Density Estimation and Importance Sampling. We establish the theoretical properties of the proposed metric, and demonstrate its superior performance in terms of variance reduction, accuracy, and quality of embeddings on real-world data. A key observation is that I-SEA shows low variance, while conventional Importance Sampling estimators are known to be unstable and result in high variance if the distribution over desired region has a small support (Precup 2000).

Limitations and Future Work. Expected Alignment for estimating the distance requires additional sampling and distance computations, which add to the computational overhead in practice at the training stage. Nevertheless, we demonstrate that the learned embeddings lead to better performance, while capturing the geometry of the data and maintaining the order of time and sample complexity. Although I-SEA can handle irregular sampling in time-series, a detailed exploration along with strategies to address missing data challenge remains an open problem while also considering statistical metrics (Fawaz et al. 2019). Further, estimating high-dimensional distribution $p(\cdot)$ by leveraging recent work on sampling from rare distributions (with significantly more data) also provides exciting avenues for future explorations (O’Kelly et al. 2018).

Conclusions. Learning meaningful representations from time-series data is challenging due to the difficulty in constructing a valid distance metric, and the high-dimensionality of the underlying distribution. In this work, we present a way to tackle the high-dimensionality via Importance Sampling for effectively leveraging the inherent structure for various machine learning tasks. Our flexible framework can serve as a general recipe for future explorations, and for learning distribution-aware embeddings for multi-variate time-series.
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sequence matching. *IEEE transactions on pattern analysis and machine intelligence*.


Supplementary Material for
I-SEA: Importance Sampling and Expected Alignment-based Deep Distance Metric
Learning for Time Series Analysis and Embedding

A Proofs of Theoretical Results

A.1 Proof of Theorem [1]

**Proof.** Non-negativity: For a distance metric \(d(\cdot)\), from Definitions 2.2 and 2.3 we have that

\[
D_{I-SEA}(X, Y) = \sum_{U \in \{U_t\}} f(U) \sum_{A_U \in A_U} \sum_{t=1}^{T} d(X_{a_U}(t), Y_{b_U}(t))p(A_U) \geq 0,
\]

since \(d(X_{a_U}(t), Y_{b_U}(t)) \geq 0\).

Symmetry: Again, since \(d(\cdot)\) is a valid distance metric from Definitions 2.2 and 2.3 we have that

\[
D_{I-SEA}(X, Y) = D_{I-SEA}(Y, X).
\]

Triangle Inequality: For the following discussion, for a time-series of length of \(T\) let \(A(T, U)\) denote the set of alignment paths of length \(U\). Now, from Definition 2.3 we have that

\[
D_{I-SEA}(X, Y) = \sum_{U \in \{U_t\}} f(U) \sum_{A_U \in A_U} D^{X,Y}_{A_U} p(A_U),
\]

\[
= \sum_{U \in \{U_t\}} f(U) \sum_{a \in A(T_x, U)} \sum_{b \in A(T_y, U)} D^{X,Y}_{a,b} p(a, b).
\]

Therefore, by marginalizing over \(c\) and \(a\),

\[
= \sum_{c \in A(T_x, U)} \sum_{b \in A(T_y, U)} \sum_{a \in A(T_x, U)} D^{X,Y}_{a,b} p(a, b, c) + \sum_{c \in A(T_x, U)} \sum_{b \in A(T_y, U)} \sum_{a \in A(T_x, U)} D^{Z,Y}_{c,b} p(a, b, c),
\]

\[
= \sum_{c \in A(T_x, U)} \sum_{b \in A(T_y, U)} \sum_{a \in A(T_x, U)} p(a, b, c) \left( D^{X,Y}_{a,b} + D^{Z,Y}_{c,b} \right),
\]

\[
\geq \sum_{c \in A(T_x, U)} \sum_{b \in A(T_y, U)} \sum_{a \in A(T_x, U)} \sum_{t=1}^{U} d(X_{a_U}(t), Y_{b_U}(t)) + \sum_{c \in A(T_x, U)} \sum_{b \in A(T_y, U)} \sum_{a \in A(T_x, U)} \sum_{t=1}^{U} d(X_{a_U}(t), Z_{c_U}(t)),
\]

\[
\sum_{c \in A(T_x, U)} \sum_{b \in A(T_y, U)} \sum_{a \in A(T_x, U)} p(a, b, c) D^{X,Z}_{a,c},
\]

where we use marginalization over \(b\) in the last step. Finally, multiplying both sides by \(f(U)\) and summing over \(U \in \{U_t\}\) concludes the proof.

A.2 Proof of Lemma [2]

**Proof.** Let \(q(\cdot)\) denote the distribution we can acquire samples with (this can be Uniform distribution for example), then we can write

\[
D_{I-SEA}(X, Y) = \sum_{U \in \{U_t\}} f(U) \sum_{A_U \in A_U} D^{X,Y}_{A_U} p(A_U),
\]
\[ D_{I-SEA}(X, Y) = \sum_{U \in \{U_1, U_2\}} f(U) \sum_{A_U \in \mathcal{A}_U} D_{A_U}(X, Y) \frac{p(A_U)}{q(A_U)}, \]
\[ = \mathbb{E}_{U \sim \mathcal{U}(U_1, U_2)} \left[ \mathbb{E}_{A_U \sim q(A_U)} \left[ D_{A_U}(X, Y) \frac{p(A_U)}{q(A_U)} \right] \right] \]  
\[ (1) \]

**A.3 Proof of Lemma 3**

*Proof.* Consider the empirical estimate \( \hat{D}_{I-SEA} \), taking expectation w.r.t. alignment paths \( A_U \), and lengths \( U \), we have
\[ \mathbb{E}_U \left[ \mathbb{E}_{A_U} \left[ \hat{D}_{I-SEA} \right] \right] = \mathbb{E}_U \left[ \mathbb{E}_{A_U} \left[ \frac{1}{m} \sum_{i=1}^{m} D_{A_i}(X, Y) \frac{p(A_i)}{q(A_i)} \right] \right]. \]  
(2)

Since alignment paths are drawn independently, we have
\[ \mathbb{E}_U \left[ \mathbb{E}_{A_U} \left[ \hat{D}_{I-SEA} \right] \right] = \frac{1}{m} \sum_{i=1}^{m} \mathbb{E}_U \left[ \mathbb{E}_{A_i} \left[ D_{A_i}(X, Y) \frac{p(A_i)}{q(A_i)} \right] \right] = \mathbb{E}_U \left[ \mathbb{E}_{A_i} \left[ D_{A_i}(X, Y) \frac{p(A_i)}{q(A_i)} \right] \right]. \]  
(3)

Now, let \( \frac{p(A_i)}{q(A_i)} \leq \mu \), where \( \mu = \mathcal{O}(1) \). This assumption ensures that the discrepancy between \( p(A_i) \) and \( q(A_i) \) is bounded.

Now, since the local distances are bounded by 1 and we have that
\[ 0 \leq D_{A_i}(X, Y) \frac{p(A_i)}{q(A_i)} \leq U_h \mu. \]

Using Hoeffding’s inequality (Hoeffding [1994]) we have
\[ \mathbb{P} \left[ |\hat{D}_{I-SEA} - D_{I-SEA}| \geq \epsilon \right] \leq 2 \exp \left( -2m \frac{\epsilon^2}{4 \mu^2} \right). \]

Now, let
\[ 2 \exp \left( -2m \frac{\epsilon^2}{4 \mu^2} \right) \leq \delta \]
for some target tolerance \( \delta \), then we need
\[ m \geq \frac{U_h^2 \mu^2}{2 \delta} \log \left( \frac{2}{\delta} \right). \]

For instance to setting \( \delta = \mathcal{O}(\exp \left( -\frac{1}{4} \right)) \) we will require \( m = \Omega \left( \frac{U_h^2 \mu^2}{\delta^2} \right) \). Finally, this implies that
\[ \mathbb{P} \left[ |\hat{D}_{I-SEA} - D_{I-SEA}| \leq \epsilon \right] \geq 1 - \delta, \]
which proves the result. Note that this analysis directly applies to Weighted Importance Sampling variant as well.

**B Algorithm for Uniform Sampling over Alignment Paths**

The algorithm for uniformly sampling over all alignment paths is shown in Algorithm B.1. For irregular time series, the sampling step for \( \alpha_U \) and \( \beta_U \) can be restricted to the available time-steps instead of \( \mathbb{N}^{T_X} \) and \( \mathbb{N}^{T_Y} \), respectively.

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1 Such an assumption is at the core of all Importance Sampling (IS) based estimation procedures. Specifically, one of the key assumptions in Importance Sampling is that for a function \( F(X) \),
\[ \mathbb{E}_p[F(X)] = \int F(x)p(x)dx, \]
can be estimated using a distribution \( q(\cdot) \) as
\[ \mathbb{E}_q[F(X)] = \mathbb{E}_q[F(X)p(X)]. \]
if \( q(\cdot) = 0 \) implies that \( F(\cdot)p(\cdot) = 0 \). In other words, \( q(\cdot) > 0 \) if \( F(\cdot)p(\cdot) \neq 0 \); hence our upper-bound (Rubinstein and Kroese [2016]). Further, this ratio is also reminiscent of the Kullback-Leibler divergence between the two distributions. In practice, closer the two distributions, the better the performance of the IS-based estimator, which is the primary motivation for opting for parametric and non-parametric methods (Zhang [1996]).
Algorithm B.1: Uniform Sampling of Alignment Paths

**Input**: Multi-variate time-series \( X \in \mathbb{R}^{n\times T_X} \) and \( Y \in \mathbb{R}^{n\times T_Y} \), and alignment path length limits \( U_L \) and \( U_H \).

**Output**: Sampled alignment path \( A_U := (\alpha_U, \beta_U) \).

1. Sample alignment path length \( U \sim U\{U_L, U_H\} \).
2. Sample \( \alpha_U \in N^{T_X} \) and \( \beta_U \in N^{T_Y} \) independently such that

   \[ \sum_{i=1}^{T_X} \alpha_i = U \quad \text{and} \quad \sum_{j=1}^{T_Y} \beta_j = U \]

   where element \( \alpha_i \) of vector \( \alpha \in N^{T_X} \), indicates the number of times the \( i \)-th time-step of \( X \) is repeated in \( \alpha_U \), and likewise for vector \( \beta \in N^{T_Y} \); see also Che et al. (2017) Pg. 3 Sec. 3.1.

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**Figure C.1**: Visualizing raw data via embeddings. Panels (a), (b), and (c) show the raw embeddings for UCI-EEG (32), UCI-EEG (64), and the PhysioNet dataset, respectively. For each of these panels (i), (ii), and (iii) correspond to embedding to a 2-D space via Principal Component Analysis (PCA), Multidimensional Scaling (MDS), and t-distributed Stochastic Neighbor Embedding (t-SNE), respectively. Green and red denote the two classes in the dataset. (Best viewed in color.)

**C Detailed Results**

**C.1 Experimental Details**

**Pre-processing** We standardize the data such that the resulting dataset is normalized to have zero-mean and unit variance across the features/variables. In addition, since the observations are recorded irregularly in case of the PhysioNet Dataset, there are a number of missing entries. To this end, we use mean-based missing value imputation scheme. In addition, if multiple values were observed for a variable in an hour, we use their mean to form the observation for that hour. Fig. C.1 shows the embeddings of the raw data using Principal Component Analysis (PCA), Multidimensional Scaling (MDS), and t-distributed Stochastic Neighbor Embedding (t-SNE).
Baselines  We use the following similarity and distance metric measures to evaluate the performance of I-SEA for the metric learning tasks on the aforementioned datasets. These include both data independent and dependent methods.

1. MDTW: Multivariate Dynamic Time Warping (MDTW) is a popular variant of Dynamic Time Warping (DTW) for multivariate time-series alignment and similarity computation. This is a data-independent technique, and is not a valid metric.

2. MDTW-NN: A neural network-based MDTW technique and hence can be viewed as a data-dependent counterpart of MDTW. The method computes the MDTW similarity measure in the transformed space.

3. GAK: Global Alignment Kernel is a data-independent metric which uses a positive semi-definite kernel to measure all similarities between time-series enabled by the kernel-trick (Cuturi [2011] Cuturi et al. [2007]). We follow the recommendation of the authors to set the hyper-parameters for our experiments.

4. Decade: is an Expected Alignment based distance metric which samples the alignment paths uniformly to estimate the distance between time-series (Che et al. [2017]). This metric is used in conjunction with a neural network, therefore serves as a baseline for deep metric learning with Expected Alignment.

5. Soft-DTW We use a neural network-based Soft-DTW is a differentiable DTW variant which can be used as a regularizer for training, it computes a soft minimum over all alignment paths (Cuturi and Blondel [2017]).

6. Ma-NN or Manhattan Neural Network baselines is based on the Siamese architectures proposed by Mueller and Thayagarajan [2016]. This models compares the Manhattan-based \( \ell_1 \) distance metric between the learned representations to compare the
Appendix C.1 for the UCI-EEG workshop on mining and learning from time series PhysioNet Dataset. The learned embeddings for the PhysioNet dataset across various methods are shown in Fig. C.3.

K-Nearest Neighbour Accuracy results and Learned Embeddings for PhysioNet Dataset

Table C.3: K-Nearest Neighbour Accuracy for the PhysioNet dataset

<table>
<thead>
<tr>
<th>Method</th>
<th>$K = 1$</th>
<th>$K = 3$</th>
<th>$K = 5$</th>
<th>$K = 7$</th>
<th>$K = 9$</th>
<th>$K = 11$</th>
<th>$K = 13$</th>
<th>$K = 15$</th>
<th>$K = 17$</th>
<th>$K = 19$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I-SEA (WIS-KDE)</td>
<td>0.659 ± 0.011</td>
<td>0.673 ± 0.007</td>
<td>0.673 ± 0.006</td>
<td>0.673 ± 0.01</td>
<td>0.676 ± 0.016</td>
<td>0.671 ± 0.009</td>
<td>0.672 ± 0.009</td>
<td>0.671 ± 0.007</td>
<td>0.671 ± 0.004</td>
<td>0.671 ± 0.002</td>
</tr>
<tr>
<td>I-SEA (WIS-Unif)</td>
<td>0.652 ± 0.016</td>
<td>0.666 ± 0.025</td>
<td>0.672 ± 0.026</td>
<td>0.672 ± 0.03</td>
<td>0.672 ± 0.023</td>
<td>0.674 ± 0.021</td>
<td>0.672 ± 0.028</td>
<td>0.668 ± 0.029</td>
<td>0.669 ± 0.028</td>
<td>0.670 ± 0.028</td>
</tr>
<tr>
<td>Decade</td>
<td>0.651 ± 0.029</td>
<td>0.671 ± 0.024</td>
<td>0.668 ± 0.028</td>
<td>0.669 ± 0.023</td>
<td>0.660 ± 0.028</td>
<td>0.667 ± 0.032</td>
<td>0.669 ± 0.029</td>
<td>0.672 ± 0.012</td>
<td>0.670 ± 0.031</td>
<td>0.671 ± 0.034</td>
</tr>
<tr>
<td>Soft-DTW</td>
<td>0.622 ± 0.046</td>
<td>0.636 ± 0.031</td>
<td>0.635 ± 0.031</td>
<td>0.636 ± 0.032</td>
<td>0.629 ± 0.031</td>
<td>0.629 ± 0.033</td>
<td>0.628 ± 0.031</td>
<td>0.629 ± 0.034</td>
<td>0.628 ± 0.034</td>
<td></td>
</tr>
<tr>
<td>MDTW-NN</td>
<td>0.642 ± 0.032</td>
<td>0.648 ± 0.036</td>
<td>0.655 ± 0.026</td>
<td>0.659 ± 0.023</td>
<td>0.643 ± 0.021</td>
<td>0.646 ± 0.018</td>
<td>0.641 ± 0.020</td>
<td>0.643 ± 0.018</td>
<td>0.643 ± 0.021</td>
<td></td>
</tr>
<tr>
<td>Ma-NN</td>
<td>0.641 ± 0.024</td>
<td>0.634 ± 0.021</td>
<td>0.650 ± 0.019</td>
<td>0.648 ± 0.017</td>
<td>0.655 ± 0.021</td>
<td>0.653 ± 0.022</td>
<td>0.654 ± 0.021</td>
<td>0.654 ± 0.025</td>
<td>0.652 ± 0.025</td>
<td></td>
</tr>
<tr>
<td>MDTW</td>
<td>0.621 ± 0.015</td>
<td>0.632 ± 0.020</td>
<td>0.643 ± 0.030</td>
<td>0.664 ± 0.039</td>
<td>0.660 ± 0.040</td>
<td>0.652 ± 0.035</td>
<td>0.645 ± 0.046</td>
<td>0.647 ± 0.039</td>
<td>0.650 ± 0.040</td>
<td></td>
</tr>
<tr>
<td>GAK</td>
<td>0.613 ± 0.012</td>
<td>0.633 ± 0.023</td>
<td>0.648 ± 0.022</td>
<td>0.655 ± 0.031</td>
<td>0.654 ± 0.041</td>
<td>0.649 ± 0.033</td>
<td>0.649 ± 0.040</td>
<td>0.644 ± 0.027</td>
<td>0.650 ± 0.030</td>
<td></td>
</tr>
<tr>
<td>MSA</td>
<td>0.622 ± 0.012</td>
<td>0.631 ± 0.022</td>
<td>0.645 ± 0.026</td>
<td>0.662 ± 0.030</td>
<td>0.660 ± 0.038</td>
<td>0.649 ± 0.039</td>
<td>0.644 ± 0.049</td>
<td>0.630 ± 0.038</td>
<td>0.651 ± 0.045</td>
<td></td>
</tr>
<tr>
<td>LDMLT</td>
<td>0.632 ± 0.015</td>
<td>0.646 ± 0.031</td>
<td>0.649 ± 0.033</td>
<td>0.656 ± 0.036</td>
<td>0.668 ± 0.024</td>
<td>0.673 ± 0.015</td>
<td>0.668 ± 0.025</td>
<td>0.679 ± 0.027</td>
<td>0.678 ± 0.021</td>
<td></td>
</tr>
</tbody>
</table>

Table C.3 shows the mean and standard deviation across datasets, respectively, and use
task-dependent linear transformations only. (Best viewed in color).

![Figure C.3: Embedding PhysioNet Dataset based on pair-wise distances/similarities using Multidimensional Scaling (Cox and Cox 2008). Panels (a)-(f) show the neural network-based techniques, while panels (g)-(j) show the data-independent methods. Panel (j) shows the LDMLT-based embedding which uses task-dependent linear transformations only. (Best viewed in color).](image)

7. MSA: Multiple Sequence Alignment is a popular data-independent technique to compute distances between multivariate time-series data (Hogeweg and Hesper 1984). We use Euclidean distance for local distances.

8. LDMLT: LogDet divergence based Metric Learning with Triplets constraints is a Mahalanobis distance and DTW similarity-based data-dependent metric learning approach which uses linear transformation before similarity computation via DTW (Mei et al. 2015).

Experimental Set-up We use 5-fold stratified cross-validation to test the performance of all methods. For each fold, we run 5 training epochs with a learning rate of $10^{-3}$, and use 3 targets and 10 imposters for each sample. We set the hyper-parameters $\delta = 1$ and $\lambda = 2$. For DECADE and I-SEA, we set $[m, U_l, U_h] = [10, 32, 48]$ and $[5, 48, 60]$ for the UCI EEG and the PhysioNet datasets, respectively, and use 5 adaptive KDE steps.

C.2 Additional Learned Embeddings and Detailed K-NN Accuracy results

In this appendix, we list additional learned embeddings detailed K-Nearest Neighbor (K-NN) accuracy via the mean and standard deviation across 5-cross-validation folds corresponding to Fig. 3 and Section 3.4. The hyperparameter settings and other experimental specifics are as shown in Section 3 and Appendix C.

K-NN Accuracy results and Learned Embeddings for UCI-EEG Dataset Table C.1 and Table C.2 show the mean and standard deviation of the K-NN accuracy results across the cross-validation folds for I-SEA and the baselines shown in Appendix C.1 for the UCI-EEG (32) and UCI EEG (64) dataset, respectively. The learned embeddings for UCI EEG (32) and UCI EEG (64) dataset across various methods are shown in Fig. 4 and Fig. C.2, respectively.

K-NN Accuracy results and Learned Embeddings for PhysioNet Dataset Table C.3 shows the mean and standard deviation of the K-NN accuracy results across the cross-validation folds for I-SEA and the baselines shown in Appendix C.1 for the PhysioNet Dataset. The learned embeddings for the PhysioNet dataset across various methods are shown in Fig. C.3.

References


Cuturi, M.; Vert, J. P; Birkenes, O.; and Matsui, T. 2007. A kernel for time series based on global alignments. In IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), volume 2, II–413. IEEE.


