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Learning Representations for Time Series Clustering

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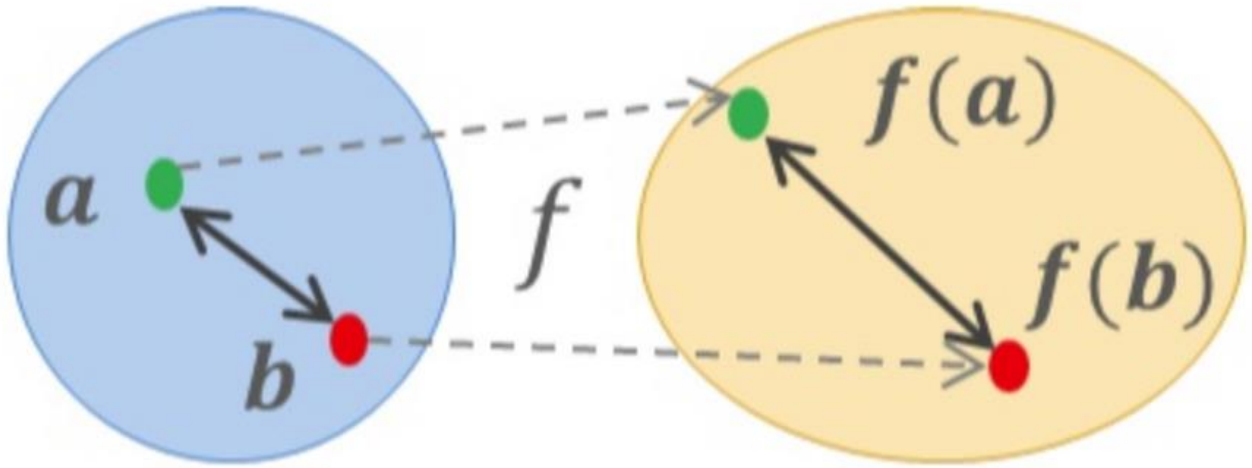
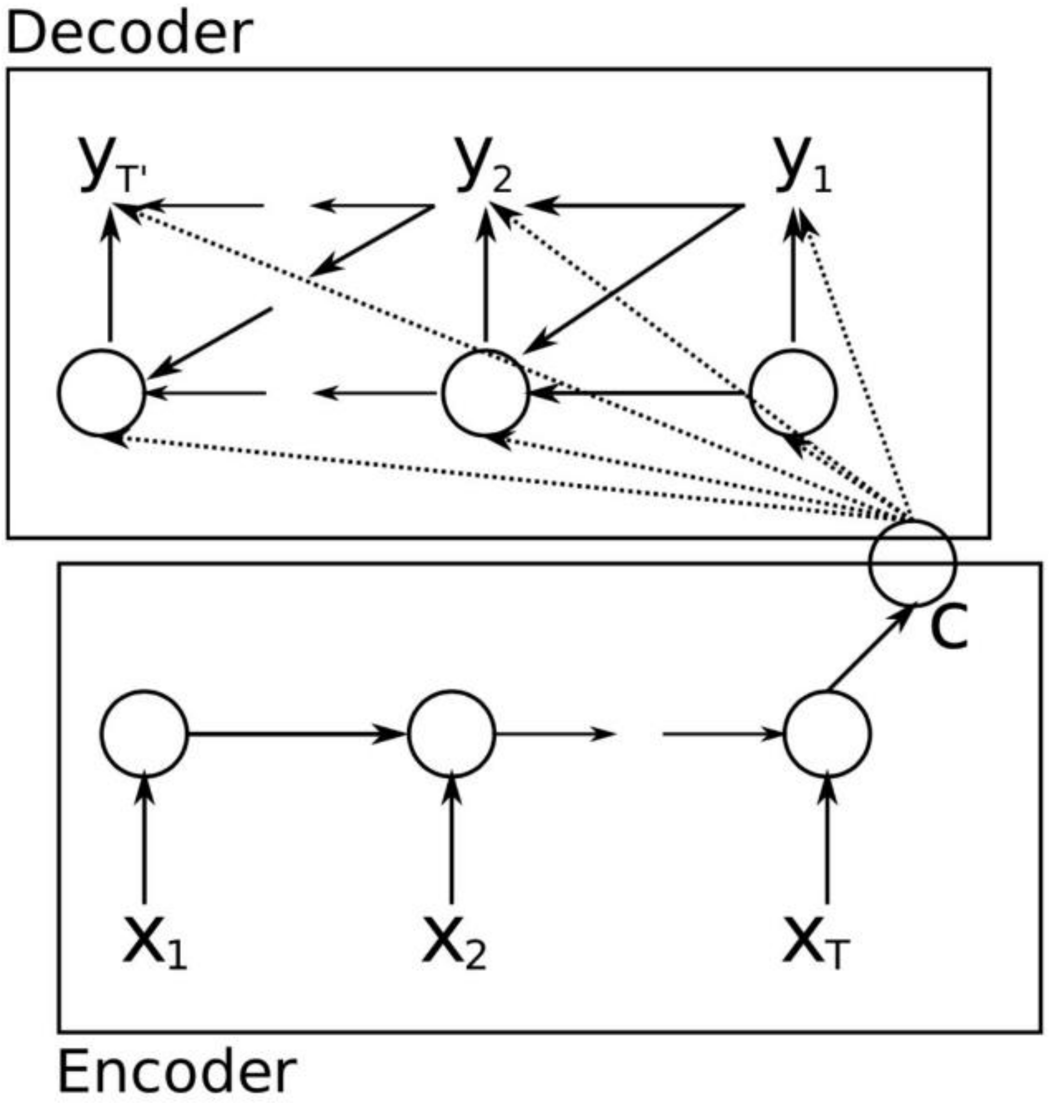
Representation Learning

> learning representations of the data that make it easier to extract useful information when building classifiers or other predictors



The representation learning of time series aims to learn a function that automatically converts the original time series into a vector representation.

Sequence to sequence (seq2seq) models



Motivation

The seq2seq model can learn general representations from sequence data in an unsupervised manner .

fine-tuned

the downstream classification task

It can significantly improve the performance. This verifies the benefits of a task-related representation.

Method---DTCR

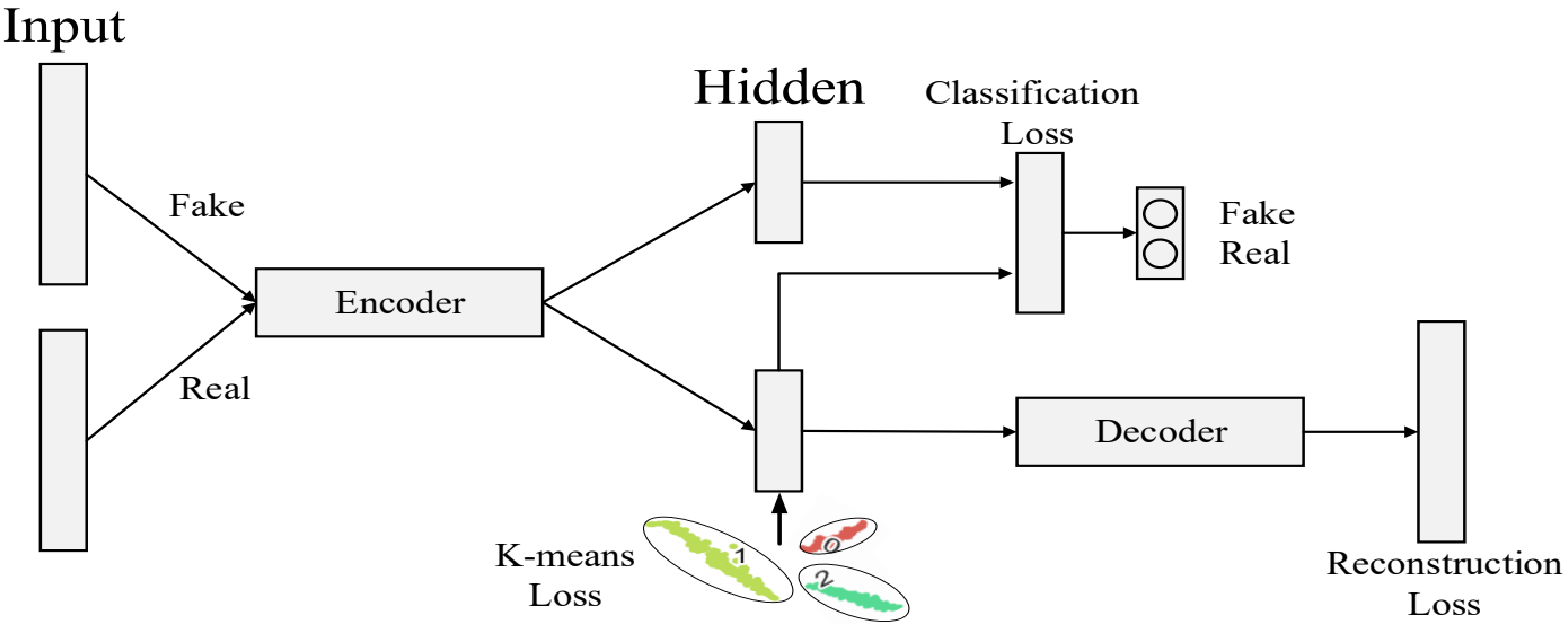


Figure 1: The general architecture of the Deep Temporal Clustering Representation (DTCR).

Method(1)---Representation Clustering

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n time series:

$$D = \{\boldsymbol{x_1}, \boldsymbol{x_2}, ..., \boldsymbol{x_n}\}$$

$$\boldsymbol{h_i} = f_{enc}(\boldsymbol{x_i})$$

$$\hat{\boldsymbol{x}}_{\boldsymbol{i}} = f_{dec}(\boldsymbol{h_i})$$

We use Mean Square Error (MSE) as the reconstruction loss:

$$\mathcal{L}_{reconstruction} = \frac{1}{n} \sum_{i=1}^{n} \| \boldsymbol{x_i} - \hat{\boldsymbol{x}}_{\boldsymbol{i}} \|_2^2$$

Method(1)---Representation Clustering

a static data matrix:

$$\boldsymbol{H} \in \mathbb{R}^{m \times N}$$

The minimization of K-means could be reformulated as a trace maximization problem associated with the Gram matrix $\boldsymbol{H}^T\boldsymbol{H}$

Spectral relaxation:

$$\mathcal{L}_{K-means} = Tr(\boldsymbol{H}^{\mathbf{T}}\boldsymbol{H}) - Tr(\boldsymbol{F}^{\mathbf{T}}\boldsymbol{H}^{\mathbf{T}}\boldsymbol{H}\boldsymbol{F})$$

$\boldsymbol{F} \in \mathbb{R}^{N \times k}$ is the cluster indicator matrix

Method(1)---Representation Clustering

$$\mathcal{L}_{K-means} = Tr(\boldsymbol{H}^{\boldsymbol{T}}\boldsymbol{H}) - Tr(\boldsymbol{F}^{\boldsymbol{T}}\boldsymbol{H}^{\boldsymbol{T}}\boldsymbol{H}\boldsymbol{F})$$

$$\max_{\boldsymbol{F}} Tr(\boldsymbol{F}^{\boldsymbol{T}}\boldsymbol{H}^{\boldsymbol{T}}\boldsymbol{H}\boldsymbol{F}),\ s.t.\ \boldsymbol{F}^{\boldsymbol{T}}\boldsymbol{F} = \boldsymbol{I}$$

The closed-form solution of F is obtained by composing the first k singular vectors of H.

$$\min_{\boldsymbol{H},\boldsymbol{F}} J(\boldsymbol{H}) + \frac{\lambda}{2}[Tr(\boldsymbol{H}^{\boldsymbol{T}}\boldsymbol{H}) - Tr(\boldsymbol{F}^{\boldsymbol{T}}\boldsymbol{H}^{\boldsymbol{T}}\boldsymbol{H}\boldsymbol{F})],\ s.t.\ \boldsymbol{F}^{\boldsymbol{T}}\boldsymbol{F} = \boldsymbol{I}$$

Fixing F, updating H can follow the standard stochastic gradient descent (SGD)
Fixing H, we update F using the closed-form solution to Eq. (5)

Method(2)---Encoder Classification Task

Given a time series $\boldsymbol{x_i} \in \mathbb{R}^T$, we generate its fake version by randomly shuffling some time steps. The number of selected time steps is $\lfloor \alpha \times T \rfloor$, where $\alpha \in (0, 1]$ is a hyper-parameter we set to 0.2.

$$\hat{\boldsymbol{y}}_{\boldsymbol{i}} = \boldsymbol{W}_{fc2}(\boldsymbol{W}_{fc1}\boldsymbol{h}_{\boldsymbol{i}})$$

$$\mathcal{L}_{classification} = -\frac{1}{2N}\sum_{i=1}^{2N}\sum_{j=1}^{2} 1\{y_{i,j} = 1\} \log \frac{\exp \hat{y}_{i,j}}{\sum_{j=1}^{2} \exp(\hat{y}_{i,j})}$$

where $\boldsymbol{y_i}$ is a 2-dim one-hot vector indicating real or fake, and $\hat{\boldsymbol{y}}_{\boldsymbol{i}}$ is the classification result. For simplicity, we ignore the bias term. $\boldsymbol{W}_{fc1} \in \mathbb{R}^{m \times d}$, $\boldsymbol{W}_{fc2} \in \mathbb{R}^{d \times 2}$ are parameters of the fully connected layers and d is set to 128.

Overall Loss Function

$$\mathcal{L}_{DTCR} = \mathcal{L}_{reconstruction} + \mathcal{L}_{classification} + \lambda \mathcal{L}_{K-means}$$

Algorithm 1 DTCR Training Method

Input: Data set: $\boldsymbol{D}$; Number of clusters: K; Alternate update: T; Maximum iterations: $MaxIter$
Output: Cluster result s

For each time series in $\boldsymbol{D}$, generate the corresponding fake samples.
for $\boldsymbol{iter} = 1$ to $MaxIter$ **do**
    Update latent representation $\{\boldsymbol{h}_i = f_{enc}(\boldsymbol{x_i})\}_{i=1}^{n}$ using SGD based on Eq. (9).
    if $\boldsymbol{iter} \;\%\; T = 0$ **then**
        Update F using the closed-form solution of Eq. (5).
    end if
end for
Apply K-means to the learned representation and get the cluster result s.

$$\boxed{\max_{\boldsymbol{F}} Tr(\boldsymbol{F^T H^T H F}),\ s.t.\ \boldsymbol{F^T F = I}}$$

Experimental Results

Data: 36 UCR time series datasets

The Rand Index (RI) :

$$RI = \frac{TP + TN}{n(n-1)/2}$$

Table 1: Rand Index (RI) comparisons on 36 time series datasets (the values in parentheses present standard deviations)

Dataset	K-means [37]	UDFS [6]	NDFS [7]	RUFS [8]	RSFS [9]	KSC [22]	KDBA [20]	k-shape [5]	u-shapelet [24]	DTC [25]	USSL [29]	DEC [26]	IDEC [27]	DTCR
Arrow	0.6905	0.7254	0.7381	**0.7476**	0.7108	0.7254	0.7222	0.7254	0.6460	0.6692	0.7159	0.5817	0.6210	0.6868(0.0026)
Beef	0.6713	0.6759	0.7034	0.7149	0.6975	0.7057	0.6713	0.5402	0.6966	0.6345	0.6966	0.5954	0.6276	**0.8046**(0.0018)
BeetleFly	0.4789	0.4949	0.5579	0.6053	0.6516	0.6053	0.6052	0.6053	0.7314	0.5211	0.8105	0.4947	0.6053	**0.9000**(0.0001)
BirdChicken	0.4947	0.4947	0.7316	0.5579	0.6632	0.7316	0.6053	0.6632	0.5579	0.4947	**0.8105**	0.4737	0.4789	**0.8105**(0.0033)
Car	0.6345	0.6757	0.6260	0.6667	0.6708	0.6898	0.6254	0.7028	0.6418	0.6695	0.7345	0.6859	0.6870	**0.7501**(0.0022)
chlorineConcentration	0.5241	0.5282	0.5225	0.5330	0.5316	0.5256	0.5300	0.4111	0.5318	0.5353	0.4997	0.5348	0.5350	**0.5357**(0.0011)
coffee	0.7460	0.8624	**1.0000**	0.5476	**1.0000**	**1.0000**	0.4851	**1.0000**	**1.0000**	0.4841	**1.0000**	0.4921	0.5767	0.9286(0.0016)
diatomsizeReduction	0.9583	0.9583	0.9583	0.9333	0.9137	**1.0000**	0.9583	**1.0000**	0.7083	0.8792	**1.0000**	0.9294	0.7347	0.9682(0.0032)
dist.phal.outl.agegroup	0.6171	0.6531	0.6239	0.6252	0.6539	0.6535	0.6750	0.6020	0.6273	0.7812	0.6650	0.7785	0.7786	**0.7825**(0.0008)
dist.phal.outl.correct	0.5252	0.5362	0.5362	0.5252	0.5327	0.5235	0.5203	0.5252	0.5098	0.5010	0.5962	0.5029	0.5330	**0.6075**(0.0024)
ECG200	0.6315	0.6533	0.6315	0.7018	0.6916	0.6315	0.6018	0.7018	0.5758	0.6018	**0.7285**	0.6422	0.6233	0.6648(0.0034)
ECGFiveDays	0.4783	0.5020	0.5573	0.5020	0.5953	0.5257	0.5573	0.5020	0.5968	0.5016	0.8340	0.5103	0.5114	**0.9638**(0.0032)
GunPoint	0.4971	0.5029	0.5102	0.6498	0.4994	0.4971	0.5420	0.6278	0.6278	0.5400	**0.7257**	0.4981	0.4974	0.6398(0.0011)
Ham	0.5025	0.5219	0.5362	0.5107	0.5127	0.5362	0.5141	0.5311	0.5362	0.5648	**0.6393**	0.5963	0.4956	0.5362(0.0035)
Herring	0.4965	0.5099	0.5164	0.5238	0.5151	0.4940	0.5164	0.4965	0.5417	0.5045	**0.6190**	0.5099	0.5099	0.5759(0.0017)
Lighting2	0.4966	0.5119	0.5373	0.5729	0.5269	0.6263	0.5119	0.6548	0.5192	0.5770	**0.6955**	0.5311	0.5519	0.5913(0.0016)
Meat	0.6595	0.6483	0.6635	0.6578	0.6657	0.6723	0.6816	0.6575	0.6742	0.3220	0.7740	0.6475	0.6220	**0.9763**(0.0016)
Mid.phal.outl.agegroup	0.5351	0.5269	0.5350	0.5315	0.5473	0.5364	0.5513	0.5105	0.5396	0.5757	0.5807	0.7059	0.6800	**0.7982**(0.0028)
Mid.phal.outl.correct	0.5000	0.5431	0.5047	0.5114	0.5149	0.5014	0.5563	0.5114	0.5218	0.5272	**0.6635**	0.5423	0.5423	0.5617(0.0006)
Mid.phal.TW	0.0983	0.1225	0.1919	0.7920	0.8062	0.8187	0.8046	0.6213	0.7920	0.7115	0.7920	0.8590	0.8626	**0.8638**(0.0007)
MoteStrain	0.4947	0.5579	0.6053	0.5579	0.6168	0.6632	0.4789	0.6053	0.4789	0.5062	**0.8105**	0.7435	0.7324	0.7686(0.0036)
OSULeaf	0.5615	0.5372	0.5622	0.5497	0.5665	0.5714	0.5541	0.5538	0.5525	0.7329	0.6551	0.7484	0.7607	**0.7739**(0.0014)
Plane	0.9081	0.8949	0.8954	0.9220	0.9314	0.9603	0.9225	0.9901	**1.0000**	0.9040	**1.0000**	0.9447	0.9447	0.9549(0.0037)
Prox.phal.outl.ageGroup	0.5288	0.4997	0.5463	0.5780	0.5384	0.5305	0.5192	0.5617	0.5206	0.7430	0.7939	0.4263	**0.8091**	**0.8091**(0.0038)
Prox.phal.TW	0.4789	0.4947	0.6053	0.5579	0.5211	0.6053	0.5211	0.5211	0.4789	0.8380	0.7282	0.8189	**0.9030**	0.9023(0.0023)
SonyAIBORobotSurface	0.7721	0.7695	0.7721	0.7787	0.7928	0.7726	0.7988	0.8084	0.7639	0.5563	0.8105	0.5732	0.6900	**0.8769**(0.0033)
SonyAIBORobotSurfaceII	0.8697	0.8745	0.8865	0.8756	0.8948	**0.9039**	0.8684	0.5617	0.8770	0.7012	0.8575	0.6514	0.6572	0.8354(0.0016)
SwedishLeaf	0.4987	0.4923	0.5500	0.5192	0.5038	0.4923	0.5500	0.5333	0.6154	0.8871	0.8547	0.8837	0.8893	**0.9223**(0.0021)
Symbols	0.8810	0.8548	0.8562	0.8525	0.9060	0.8982	**0.9774**	0.8373	0.9603	0.9053	0.9200	0.8841	0.8857	0.9168(0.0022)
ToeSegmentation1	0.4873	0.4921	0.5873	0.5429	0.4968	0.5000	0.6143	0.6143	0.5873	0.5077	**0.6718**	0.4984	0.5017	0.5659(0.0006)
ToeSegmentation2	0.5257	0.5257	0.5968	0.5968	0.5826	0.5257	0.5573	0.5257	0.5020	0.5348	0.6778	0.4991	0.4991	**0.8286**(0.0028)
TwoPatterns	0.8529	0.8259	0.8530	0.8385	**0.8588**	0.8585	0.8446	0.8046	0.7757	0.6251	0.8318	0.6293	0.6338	0.6984(0.0025)
TwoLeadECG	0.5476	0.5495	0.6328	0.8246	0.5635	0.5464	0.5476	0.8246	0.5404	0.5116	**0.8628**	0.5007	0.5016	0.7114(0.0014)
wafer	0.4925	0.4925	0.5263	0.5263	0.4925	0.4925	0.4925	0.4925	0.4925	0.5324	**0.8246**	0.5679	0.5597	0.7338(0.0006)
Wine	0.4984	0.4987	0.5123	0.5021	0.5033	0.5006	0.5064	0.5001	0.5033	0.4906	**0.8985**	0.4913	0.5157	0.6271(0.0039)
WordsSynonyms	0.8775	0.8697	0.8760	0.8861	0.8817	0.8727	0.8159	0.7844	0.8230	0.8855	0.8540	0.8893	0.8947	**0.8984**(0.0003)
AVG Rank	10.6667	9.6806	7.2222	7.3889	6.8750	7.1389	7.9167	8.2361	8.2500	8.8194	3.5000	8.6528	7.5833	**3.0694**
AVG RI	0.5975	0.6077	0.6402	0.6478	0.6542	0.6582	0.6335	0.6419	0.6402	0.6238	0.7676	0.6351	0.6515	**0.7714**
Best	0	0	1	1	1	3	2	0	1	0	12	0	1	**17**
p-value	2.089E-6	4.8823E-6	3.4131E-5	5.7729E-5	4.1222E-5	1.3545E-4	1.2565E-5	1.4814E-4	3.4141E-5	3.0287E-7	9.7386E-1	8.7697E-07	3.2916E-7	-

Ablation Study

Table 3: Rand Index (RI) ablation study results of DTCR

No.	Dataset	w/o K-means	w/o classification	DTCR	No.	Dataset	w/o K-means	w/o classification	DTCR
1	Arrow	0.5980	0.5698	**0.6868**	19	Mid.phal.outl.correct	0.5137	0.5033	**0.5617**
2	Beef	0.7352	0.6497	**0.8046**	20	Mid.phal.TW	0.8625	0.8620	**0.8638**
3	BeetleFly	0.6305	0.6053	**0.9000**	21	MoteStrain	0.7121	0.7239	**0.7686**
4	BirdChicken	0.5600	0.4821	**0.8105**	22	OSULeaf	0.7416	0.7314	**0.7739**
5	Car	0.6610	0.6688	**0.7501**	23	Plane	0.9530	0.9409	**0.9549**
6	chlorineConcentration	0.5341	0.5004	**0.5357**	24	Prox.phal.outl.ageGroup	0.8004	0.7922	**0.8091**
7	coffee	0.6672	0.5434	**0.9286**	25	Prox.phal.TW	0.8549	0.8359	**0.9023**
8	diatomsizeReduction	0.8892	0.7851	**0.9682**	26	SonyAIBORobotSurface	0.7561	0.7702	**0.8769**
9	dist.phal.outl.agegroup	0.7775	0.7780	**0.7825**	27	SonyAIBORobotSurfaceII	0.7069	0.6332	**0.8354**
10	dist.phal.outl.correct	0.5056	0.5051	**0.6075**	28	SwedishLeaf	0.9107	0.9047	**0.9223**
11	ECG200	0.6064	0.5412	**0.6648**	29	Symbols	0.8989	0.9043	**0.9168**
12	ECGFiveDays	0.6970	0.5623	**0.9638**	30	ToeSegmentation1	0.5598	0.4993	**0.5659**
13	GunPoint	0.5589	0.4969	**0.6398**	31	ToeSegmentation2	0.6878	0.6012	**0.8286**
14	Ham	0.5330	0.5040	**0.5362**	32	TwoPatterns	0.6537	0.6650	**0.6984**
15	Herring	0.5173	0.4967	**0.5759**	33	TwoLeadECG	0.5316	0.5262	**0.7114**
16	Lighting2	0.5626	0.5554	**0.5913**	34	wafer	0.5900	0.5322	**0.7338**
17	Meat	0.8245	0.7181	**0.9763**	35	Wine	0.5642	0.5159	**0.6271**
18	Mid.phal.outl.agegroup	0.7981	0.7923	**0.7982**	36	WordsSynonyms	0.8920	0.8891	**0.8984**

Visualization Analysis

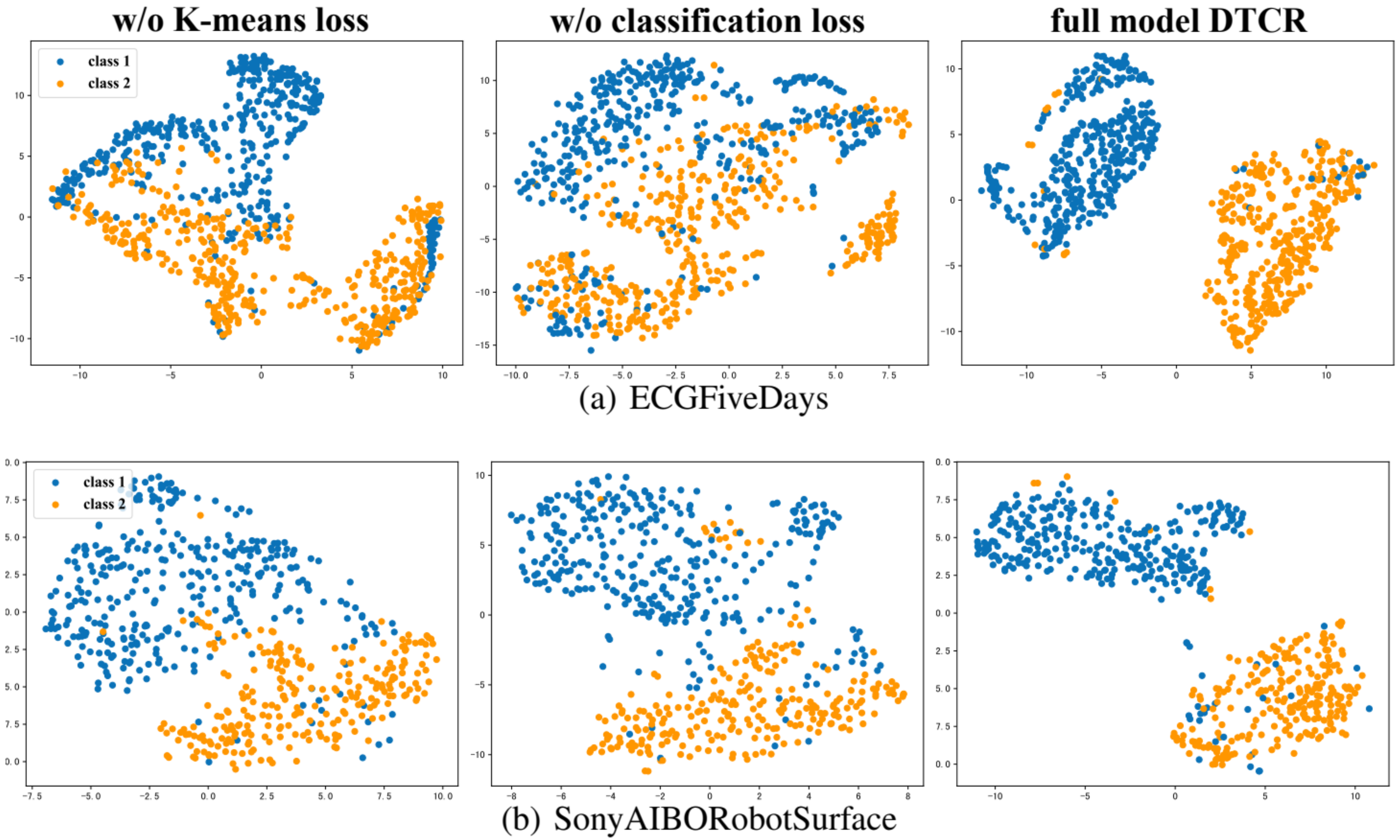


Figure 2: The visualizations with t-SNE on the datasets (a) *ECGFiveDays* and (b) *SonyAIBORobot-Surface*. The colors of the points indicate the actual labels.

The Process of Learning Representations

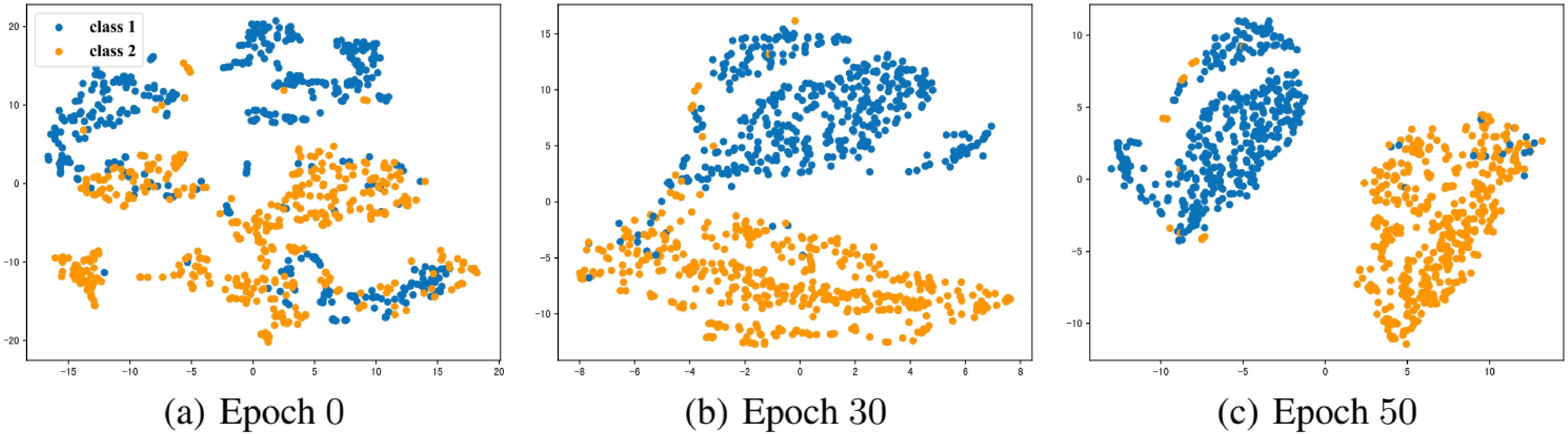
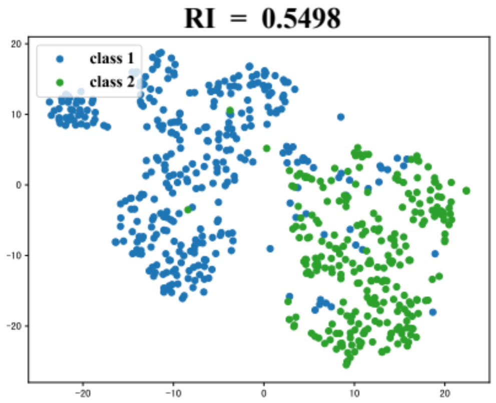
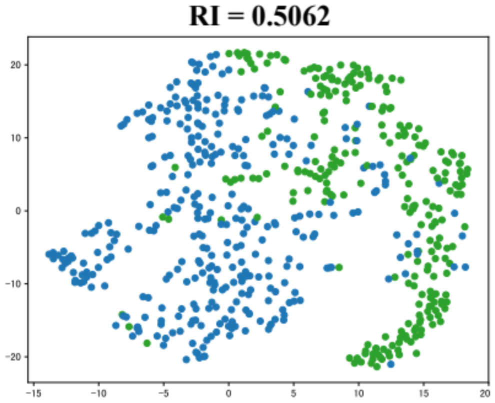


Figure 3: The learned representations on data set *ECGFiveDays* during the training process. From left to the right, the subfigure is obtained at Epoch 0, 30 and 50, respectively.

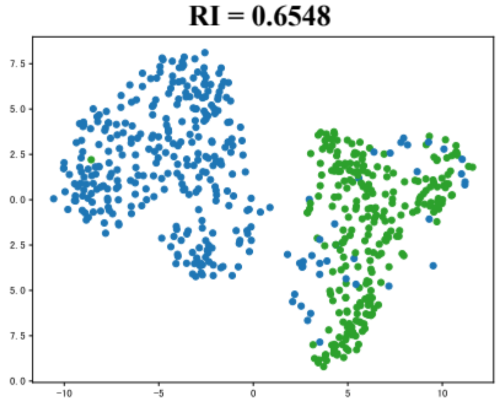
Robustness Analysis



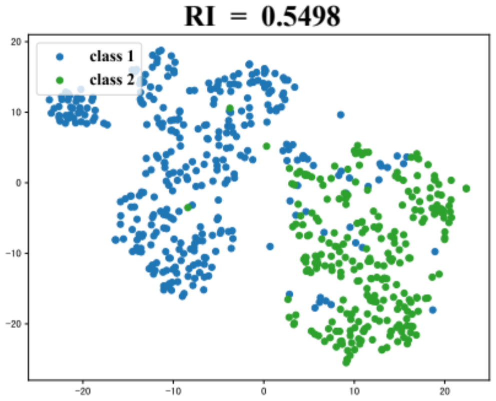
(a) Initial state



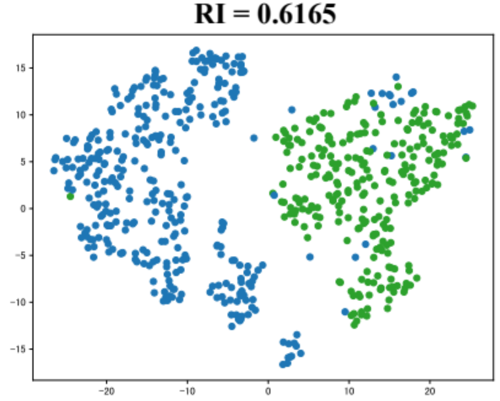
(b) Intermediate state only with shuffled K-means and classification loss



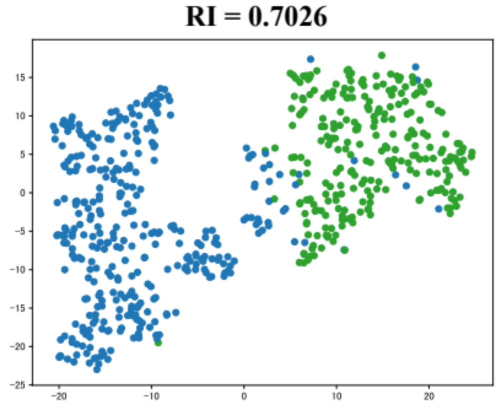
(c) Final state (putting reconstruction loss back)



(d) Initial state



(e) Intermediate state only with shuffled K-means and reconstruction loss



(f) Final state (putting classification loss back)

Figure 4: Robustness Analysis of DTCR on *SonyAIBORobotSurface*. Note that the (d) is the same as (a), replicated here for better illustration; hence the first and second rows start with the same state.

Conclusion

1. We propose a novel unsupervised temporal representation learning model for time series clustering, which integrates the temporal reconstruction and K-means objective to generate cluster-specific temporal representations.
2. We propose a fake-sample generation strategy for time series and introduce an auxiliary classification task for the encoder to enhance its ability.
3. Our experimental results on a large number of benchmark time series datasets show that the proposed model achieves state-of-the-art performance. Visualization analysis illustrates the effectiveness of cluster-specific temporal representations and demonstrates the robustness of the learning process, even if K-means makes mistakes.

THANKS