SEMI-SUPERVISED TIME-SERIES LEARNING WITH DEEP GENERATIVE MODELS

A PREPRINT

Nikita Klyuchnikov
Skoltech
nikita.klyuchnikov@skoltech.ru

Rodrigo Rivera
Skoltech
rodrigo.riveracastro@skoltech.ru

October 26, 2018

ABSTRACT

This work implements a semi-supervised approach for time series

***K*eywords** Semi-supervised, VAE, time series, learning

Contents

1 Introduction

Learning representations from data is the quintessential task in machine learning. Multiple models of different characteristics have been proposed over many decades, a recent one, based on the concept of Variational Autoencoders has found significant success across a myriad of contexts and tasks. In this report, we evaluate a further development of this model focusing on semi-supervised learning.

2 Methods

For this analysis, it was decided to make use of a series of methods for analysis and learning. A brief overview is presented below. The reader is adviced to consult the reference material for a detailed presentation of the material.

Variational Auto-Encoder Ordinary Variational Auto-Encoder (VAE) was proposed by Kingma and Welling (2014). The idea of this auto-encoding model is to approximate posterior distribution of latent parameters z with Gaussian inference network $q(z|x)$ and use it for evidence lower bound optimization. Whereas the prior is also assumed to be Gaussian $p(z) \sim \mathcal{N}(0, I)$.

Semi-Supervised Variational Auto-encoder Semi-supervised Learning with Deep Generative Models was proposed by Kingma et al. (2014), who made the following modifications to ordinary VAE:

- the dataset consists of two parts: items with supervised labels $D = \{(x_i, y^i)\}_{i=1}^{n_s}$ and unlabeled items $X = \{x_i^{(u)}\}_{i=1}^{n_u}$, for which labels are considered as additional latent variables;
- labels are generated from some categorical distribution $\text{Cat}(y|\pi)$;
- approximate posterior factorizes on Gaussian and multinational distributions of z and y:

$$q(z, y|x) = \mathcal{N}\left(z|\mu(x), \text{diag}(\sigma^2(x))\right) q(y|\pi(x))$$

These modifications lead to different training scheme, in particular, to new evidence lower bound:

$$\mathcal{J}_\alpha = \sum_{x \in X} \mathcal{U}(x) + \sum_{(x,y) \in D} \left[\mathcal{L}(x, y) - \alpha \log q(z, y|x)\right], \tag{1}$$

where $\mathcal{U}(x) = \sum_y \left[q(y|x)\left(L(x, y) - \mathbb{H}(q(y|x))\right)\right]$ and

$$L(x, y) = \mathbb{H}(q(z|x, y)) - \mathbb{E}_{q(z|x,y)}\left[\log p(x|y, z) + \log p(y) + \log p(z)\right].$$

Original paper studied the model performance on images, in this work we adjusted the model for time-series: the key difference will be in the amortized inference networks architecture, that represent $\mu(x)$, $\sigma^2(x)$ and $\pi(x)$ (see the particular architecutre that we implemented in Figure 24).

K-shape Proposed by Paparrizos and Gravano (2015). K-Shape relies on an iterative refinement procedure, which creates homogeneous clusters using a normalized version of the cross-correlation measure as its distance measure in order to consider the shapes of time series while comparing them. It also computes cluster centroids, which are used in every iteration to update the assignment of time series to clusters.

Soft-DTW A work of Cuturi and Blondel (2017) proposing a smooth version of DTW. A method that finds the optimal non-linear alignment between two time series. The traditional DTW considers two time series $Q = \{q_1, \ldots, q_n\}$ and $C = \{c_1, \ldots, c_n\}$ of the same length n. A $n \times n$ matrix is constructed, whose i, j^{th} element are the Euclidean distance between the elements q_i and c_j. The objective is to find an optimal aligment between both time series by a path through the matrix W, which minimizes the cumulative distance path. Thus, it minimizes the Euclidean distance $W^* = argmin_W(\sqrt{\Sigma_{k=1}^K w_k})$, where w_k is an element of the matrix W containing the distances between the points.

K-Means with Fast Global Alignment Kernel Presented originally by Cuturi (2011), it proposes a reformulation of DTW as toeplitz kernel. The authors show results that not only offer significantly improvements in reduction of the test error but also a faster computation.

Gaussian Mixture Model GMM is a commonly used method for clustering and density estimation. It assumes that all generated data points are derived from a mixture of a finite Gaussian distribution with unknown parameters. The parameters are often derived with methods such as maximum a posteriori (MAP).

LB-Keogh It is a popular method proposed by Keogh and Ratanamahatana (2005), to speed dynamic time warping (DTW), as the LB Keogh lower bound is linear whereas the commonly used DTW has a quadratic complexity. More concretely, LB-Keogh is defined in equation 2

$$LBKeogh(Q,C) = \Sigma_{i=1}^{n}(c_iU_i)^2 I(c_i > U_i) + (c_iL_i)2I(c_i < L_i) \tag{2}$$

where U_i and L_i are upper and lower bounds for time series Q which are defined as $U_i = max(q_{i-r} : q_{i+r})$ and $L_i = min(q_{i-r} : q_{i+r})$ for a reach r and $I(\cdot)$ is the indicator function.

Table 1: Overview of data sets used for experiments

Data set	Elements	Periods	Characteristics
Inventory demand	2400	44	Representing demand for 800+ products across 4 delivery periods. Heterogeneous demand.
MWD dataset	31352	720	Represents physical characteristics of oil-wells drilling at various stages. Long 4-d time series logs from 60 wells. Slices with length 180 periods each

Table 2: Overview of clustering methods used

Cluster method	Data set	Nr. Clusters	Notes
K-shape	Inventory demand	20	Gave the best results from all methods
K-means Kernel	Inventory demand	20	Global alignment kernel with 10 iterations. Very slow.
Soft DTW	Inventory demand	20	Method differentiable everywhere, using soft minimum gradient computed in quadratic time
GMM	Inventory demand	5	It used LB-Keogh as a distance. The results are then used to fit the GMM
K-shape	MWD	5	Slightly better results than the other methods, but with the advantage of faster computational times
Soft DTW	MWD	5	Faster than regular DTW and with similar results, but inferion vis a vis K-shape
GMM	MWD	5	

3 Exploratory data analysis

Before carrying out any learning task, a set of data sets were chosen to evaluate the suitability of the observed method for time series. On one side, a toy data set that we call *'MNIST Time series'* was generated consisting of a positive, see figure 17, and a negative, see figure 16, class. On the other side, two real data sets from commercial partners were selected. Among other reasons, a motivating factor was that they are diametrically different. One of them has long time series, consisting of 720 periods, whereas the other one consists of 44. Further, one is multi-dimensional and the other uni-dimensional. An overview of both time series is shown below in table 1.

One of the first tasks to assess if the data sets are viable to be used for a learning task was to use them for data clustering. A motivation is that the semi-supervised approach can generate predictions based on labels; a process akin to a 'hard clustering'. In addition, the heterogeneous characteristics of the data sets and the existence of corner cases (i.e., stable time series with sudden spikes) were reasons to believe that the data would pose a challenge to the semi-supervised VAE method evaluated in this work. Thus, a group of clustering algorithms were selected among the state of the art. They are summarized in table 2 and presented in section 2.

$$AdjustedRandScore = \frac{(RandScore - ExpectedRandIndex)}{[max(RandIndex) - ExpectedRandIndex]} \tag{3}$$

Further, to evaluate the different clustering methods, it was decided to use the Adjusted Rand Score as an evaluation metric, see equation 3. This is a popular metric to compare the results of a clustering task. It assess the similarities between two data clusters using the Rand Index. For a further description, the reader is invited to consult Rand (1971).

Methodology For each method proposed, a series of clusters were computed. Out of this, a centroid was obtained. This centroid is another time series. Together with th

4 Results

Toy sine-waves In this section we consider an artificial dataset with time-series in the form of sine-waves with different phases and periods. The second channel is defined by the class label: for positive class the second channel is identical to the first one (see example in Figure 17), for negative class the second channel is inverted (negation) of the first one (see example in Figure 16).

Real datasets

5 Conclusion

This projected consisted on exploring if learning representations of time series can be accomplished using variational auto-encoders (VAE). Although at first promising. The results were not satisfactory. In fact, this research argues that VAE is suboptimal for this type of data structure, specially for the case of clustering of time series. Here, it became evidently, that any run-off-the-mill clustering model achieves better results than the semi-supervised VAE model discussed in this work.

References

Cuturi, M. (2011). Fast global alignment kernels. In *Proceedings of the 28th International Conference on Machine Learning, ICML 2011, Bellevue, Washington, USA, June 28 - July 2, 2011*, pages 929–936.

Cuturi, M. and Blondel, M. (2017). Soft-dtw: a differentiable loss function for time-series. In *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*, pages 894–903.

Keogh, E. and Ratanamahatana, C. A. (2005). Exact indexing of dynamic time warping. *Knowl. Inf. Syst.*, 7(3):358–386.

Kingma, D. P., Mohamed, S., Rezende, D. J., and Welling, M. (2014). Semi-supervised learning with deep generative models. In *Advances in Neural Information Processing Systems*, pages 3581–3589.

Kingma, D. P. and Welling, M. (2014). Stochastic gradient vb and the variational auto-encoder. In *Second International Conference on Learning Representations, ICLR*.

Paparrizos, J. and Gravano, L. (2015). k-shape: Efficient and accurate clustering of time series. In *Proceedings of the 2015 ACM SIGMOD International Conference on Management of Data*, SIGMOD '15, pages 1855–1870, New York, NY, USA. ACM.

Rand, W. (1971). Objective criteria for the evaluation of clustering methods. *Journal of the American Statistical Association*, 66(336):846–850.

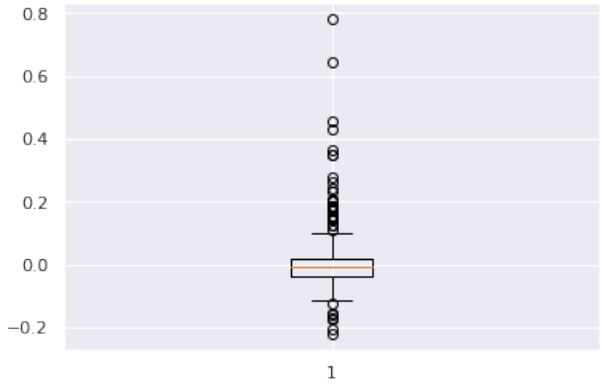

Figure 1: Boxplot of adjusted rand score of Gaussian Mixture Model for inventory demand

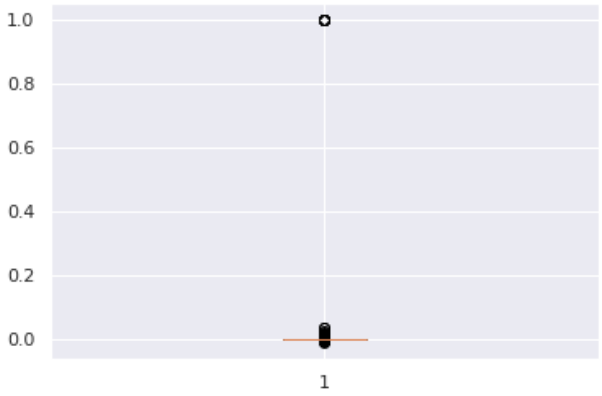

Figure 2: Boxplot of adjusted rand score of K-Shape clustering for inventory demand data set

A Appendix

Following figures were used accross this work

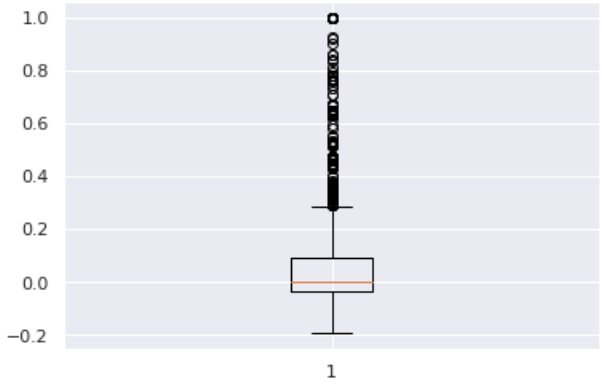

Figure 3: Boxplot of adjusted rand score of K-Means Kernel clustering for inventory demand data set

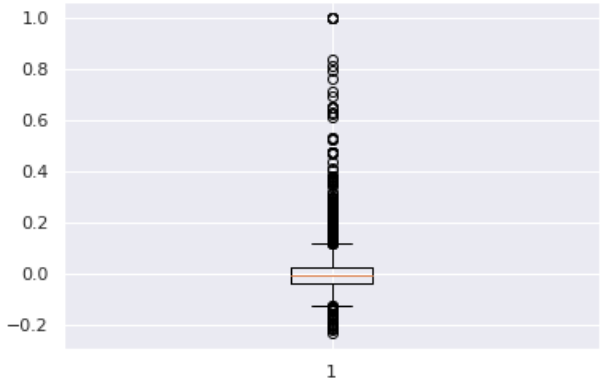

Figure 4: Boxplot of adjusted rand score of Soft-DTW Kernel clustering for inventory demand data set

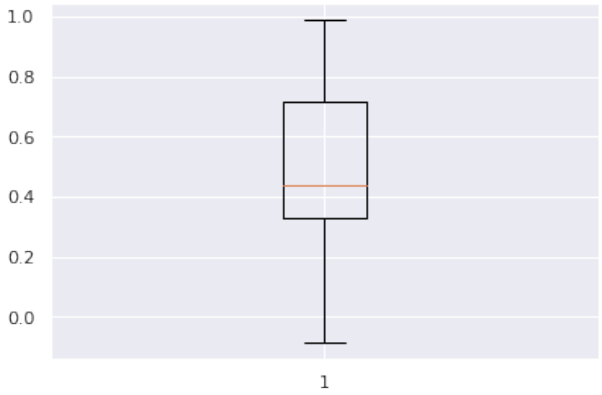

Figure 5: Boxplot of adjusted rand score of Gaussian Mixture Model for MWD data set

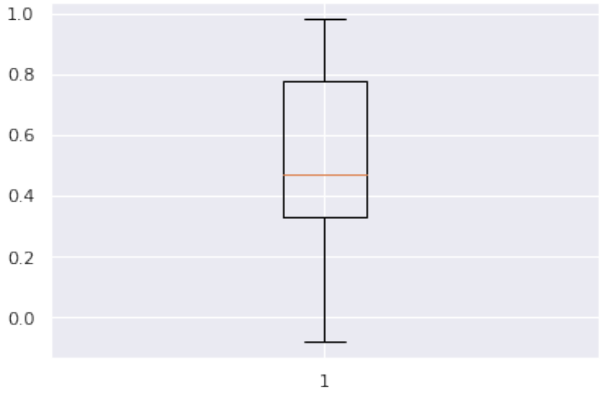

Figure 6: Boxplot of adjusted rand score of K-Shape clustering for MWD data set

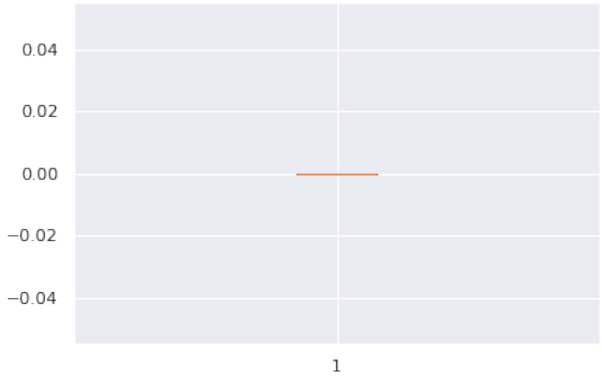

Figure 7: Boxplot of adjusted rand score of K-Means Kernel clustering for MWD data set

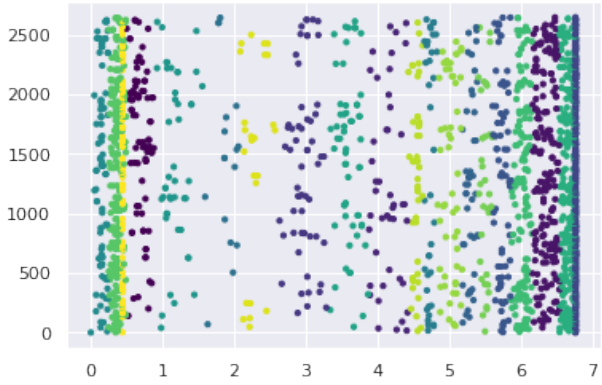

Figure 8: Clusters using Gaussian Mixture Model for inventory demand

A.1 Box Plots

A.2 Clusters

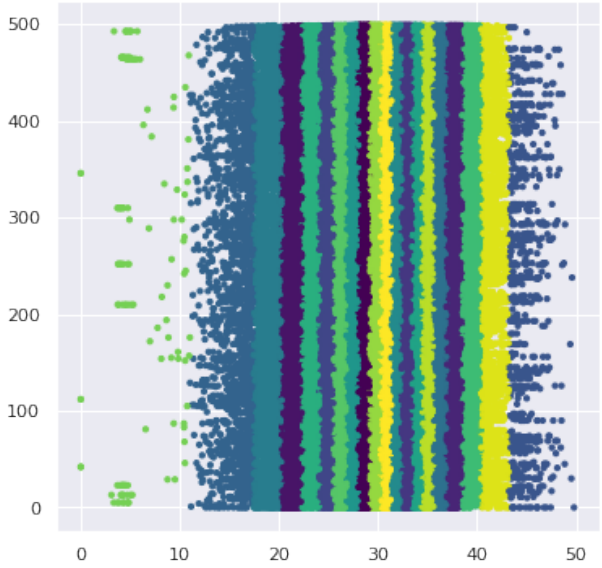

Figure 9: Clusters using Gaussian Mixture Model for MWD data set

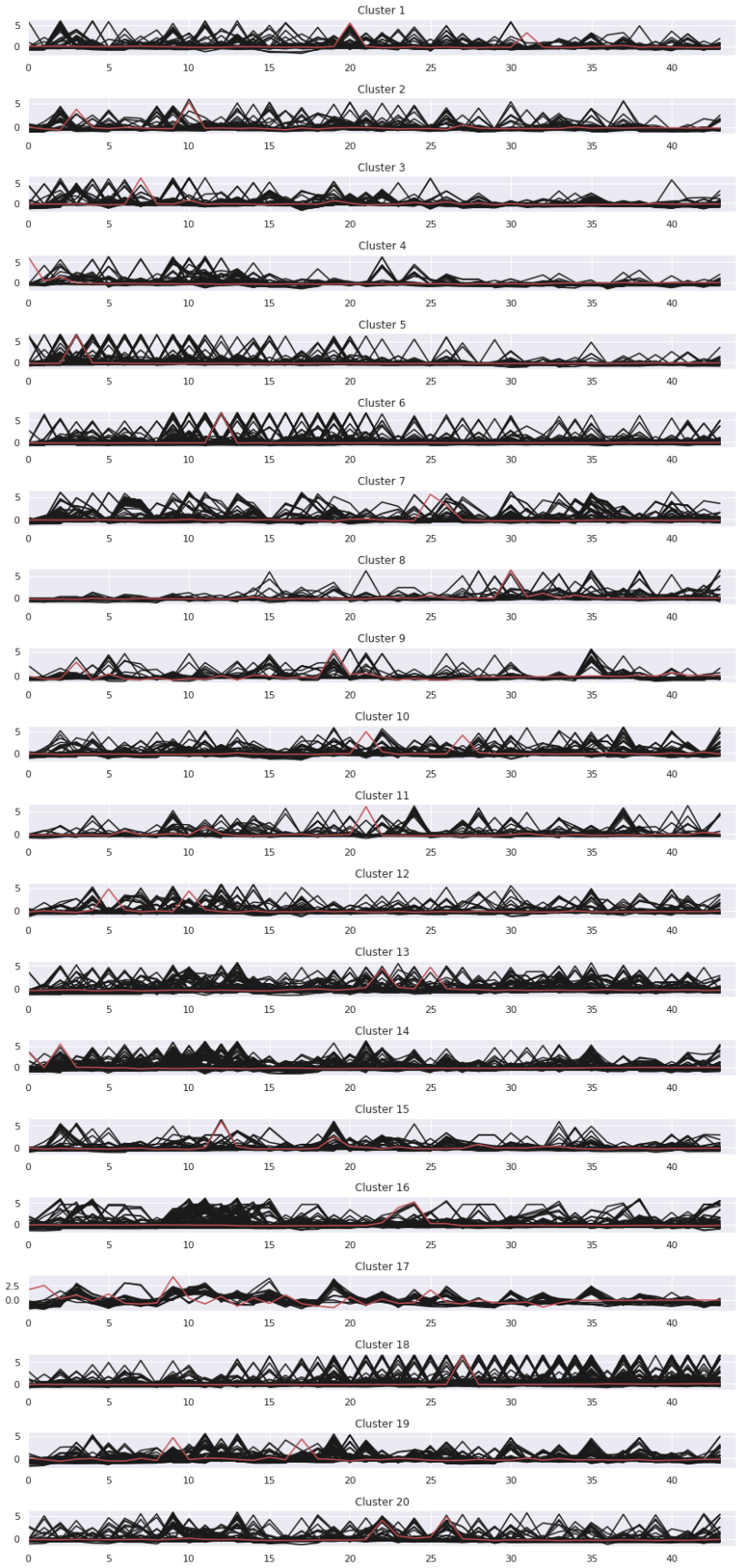

Figure 10: Clusters using K-Shape clustering for inventory demand data set

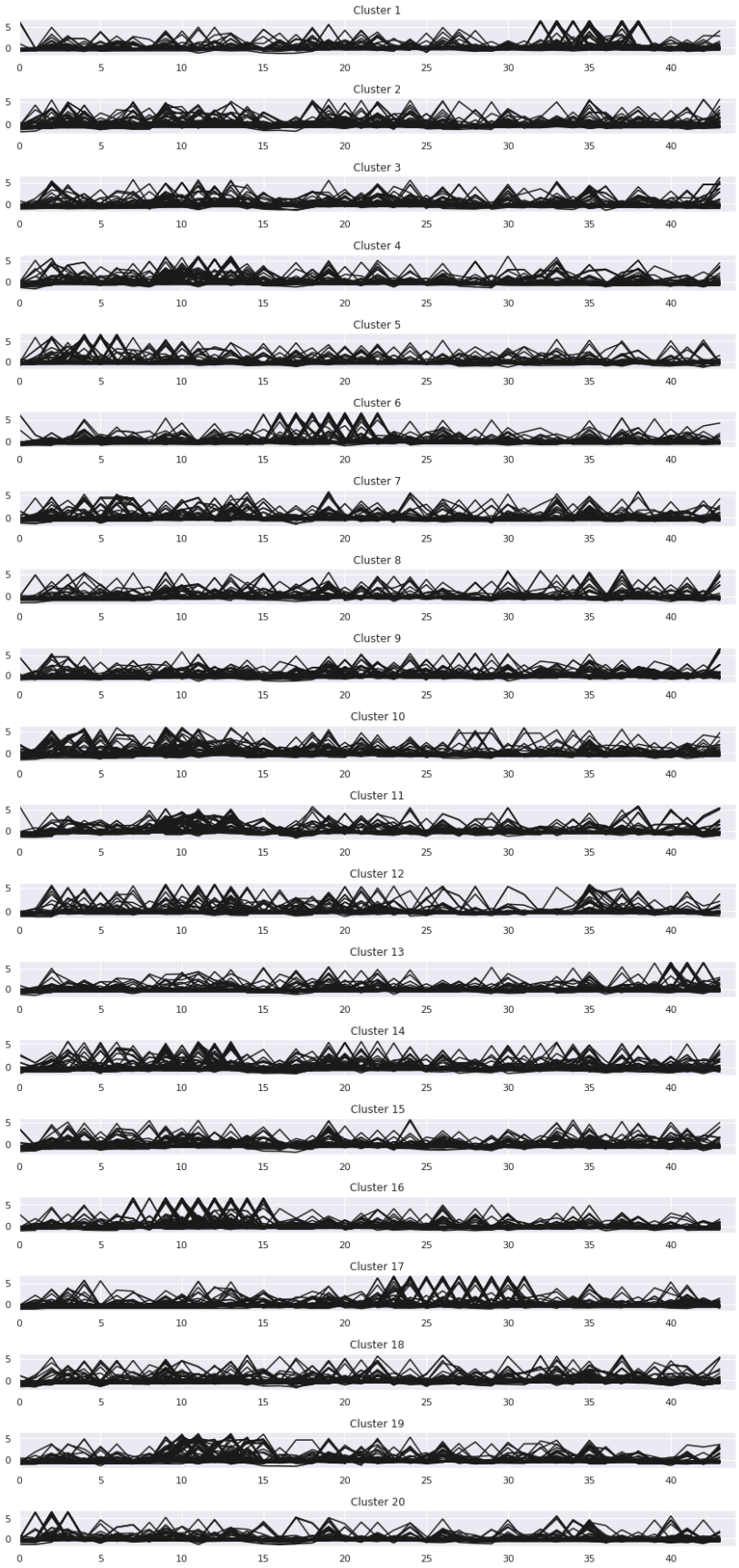

Figure 11: Clusters using K-Means Kernel clustering for inventory demand data set

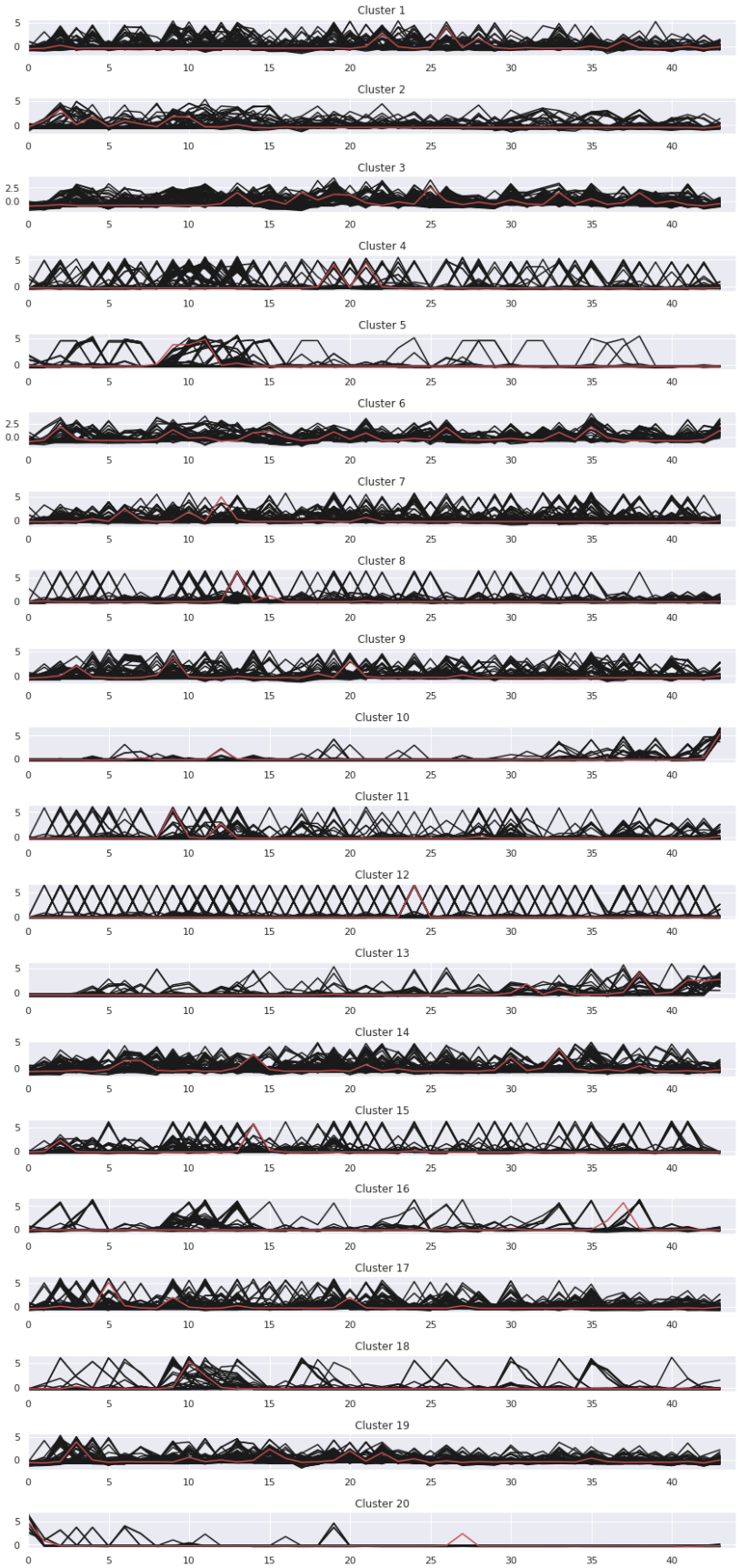

Figure 12: Boxplot of adjusted rand score of Soft-DTW Kernel clustering for inventory demand data set

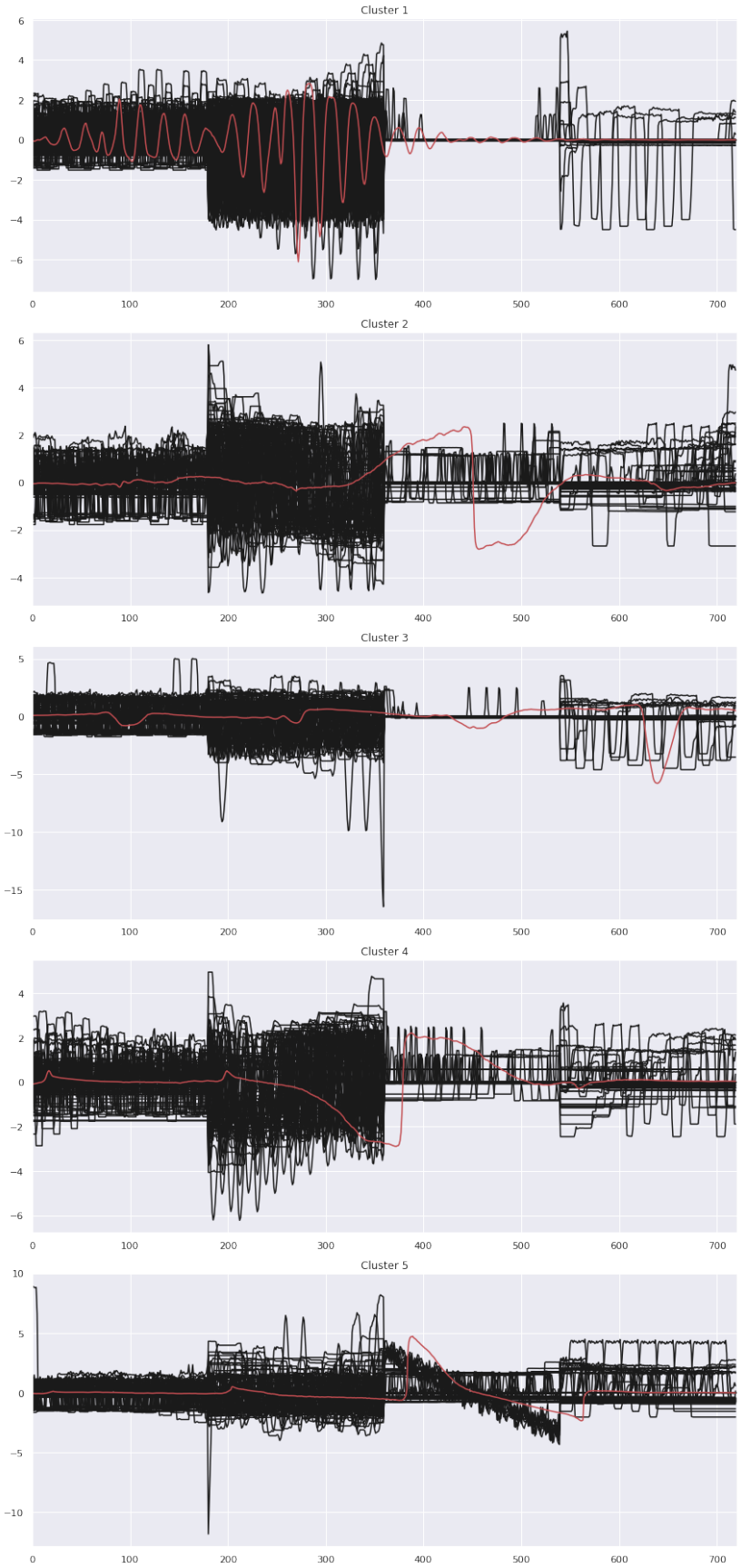

Figure 13: Clusters using K-Shape clustering for MWD data set

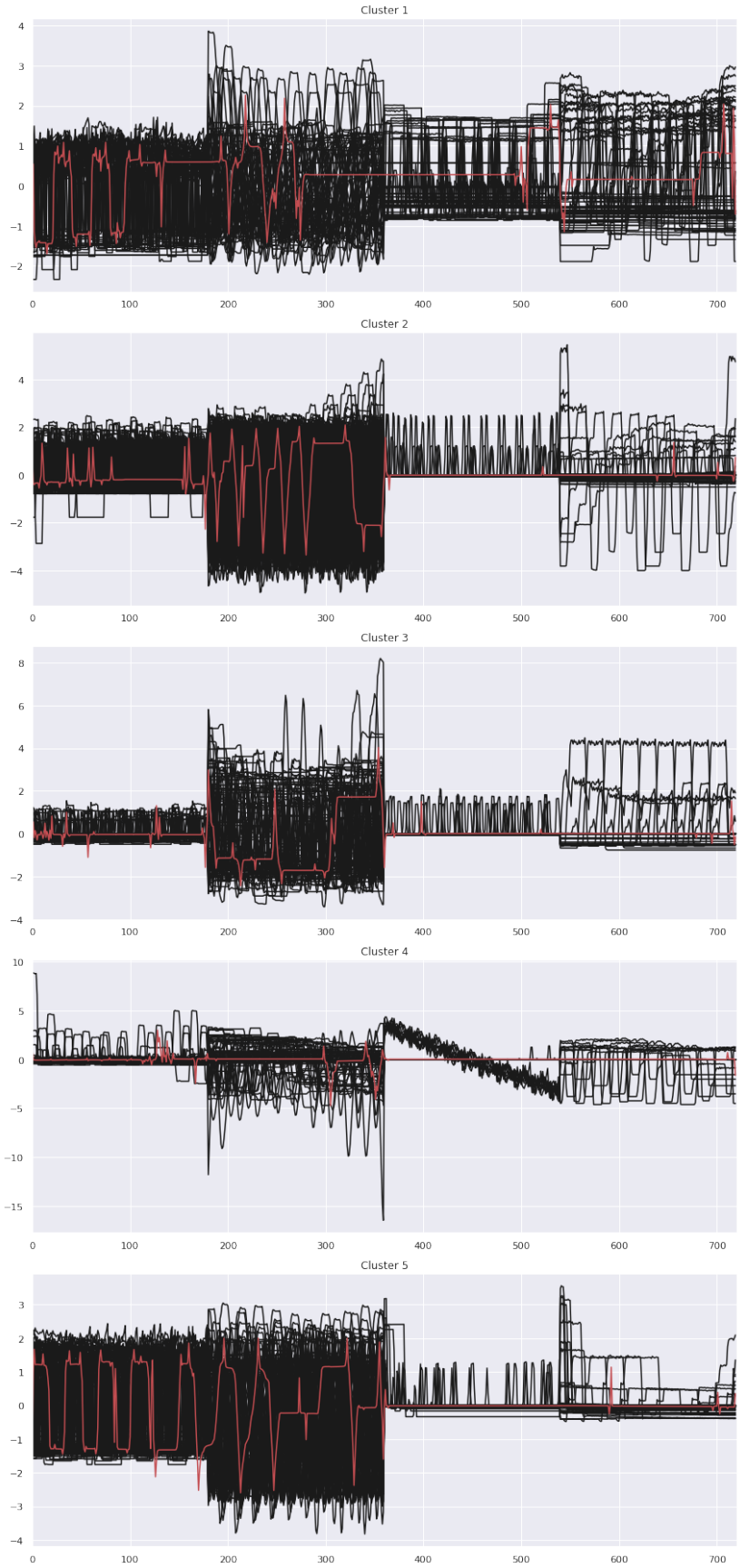

Figure 14: Clusters using K-Means Kernel clustering for MWD data set

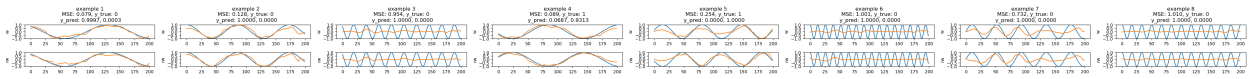

Figure 15: Semi-supervised reconstruction.

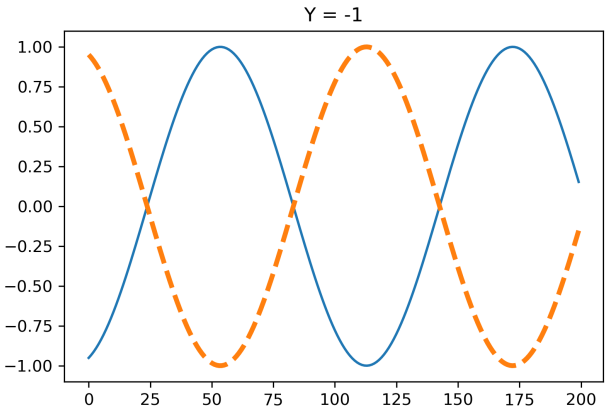

Figure 16: Negative class example.

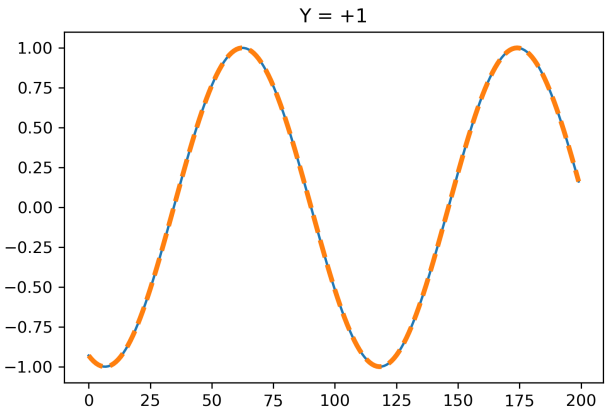

Figure 17: Positive class example.

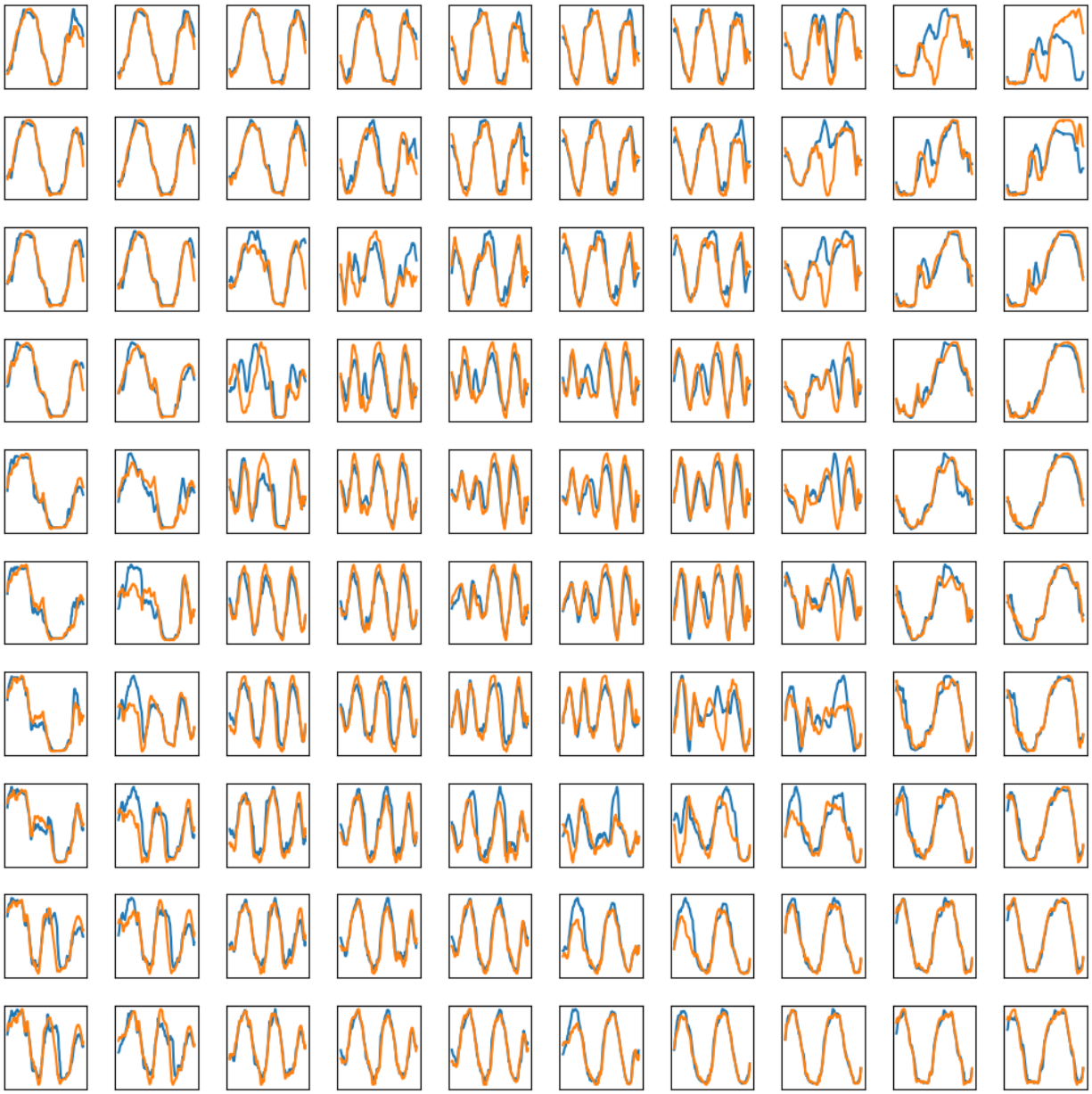

Figure 18: Exploration of latent space with positive label.

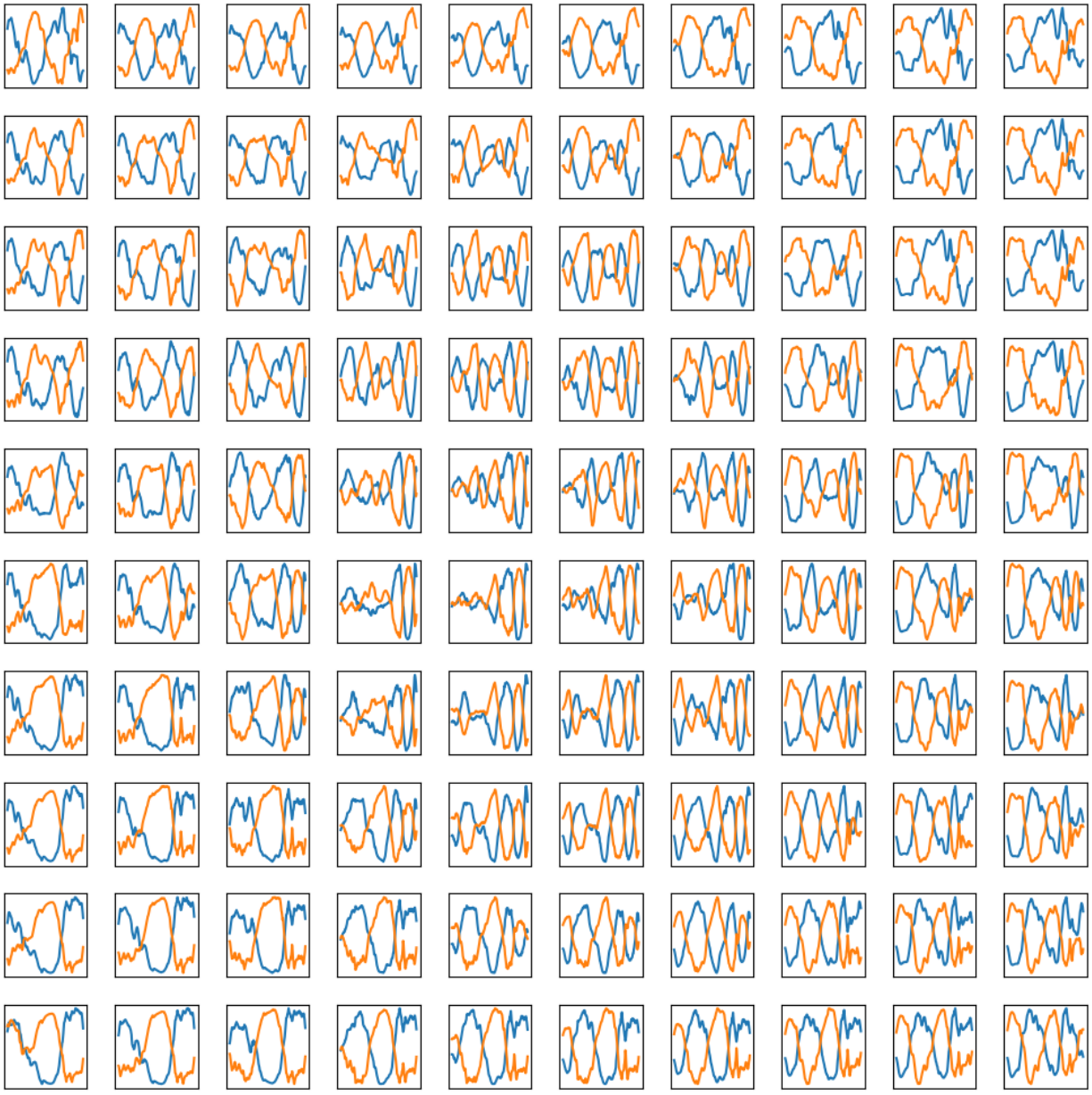

Figure 19: Exploration of latent space with negative label.

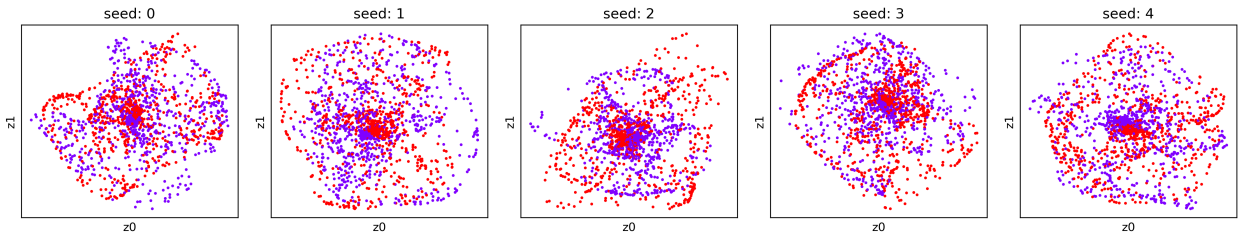

Figure 20: Semi-supervisedd latent representations.

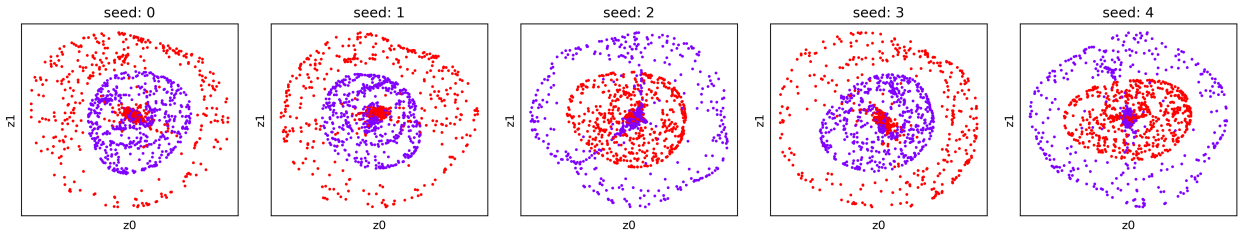

Figure 21: Unsupervised latent representations.

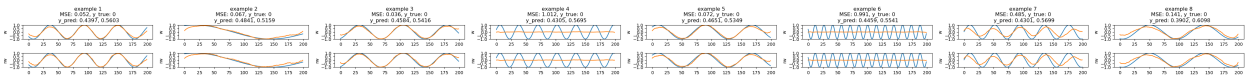

Figure 22: Unsupervised reconstruction.

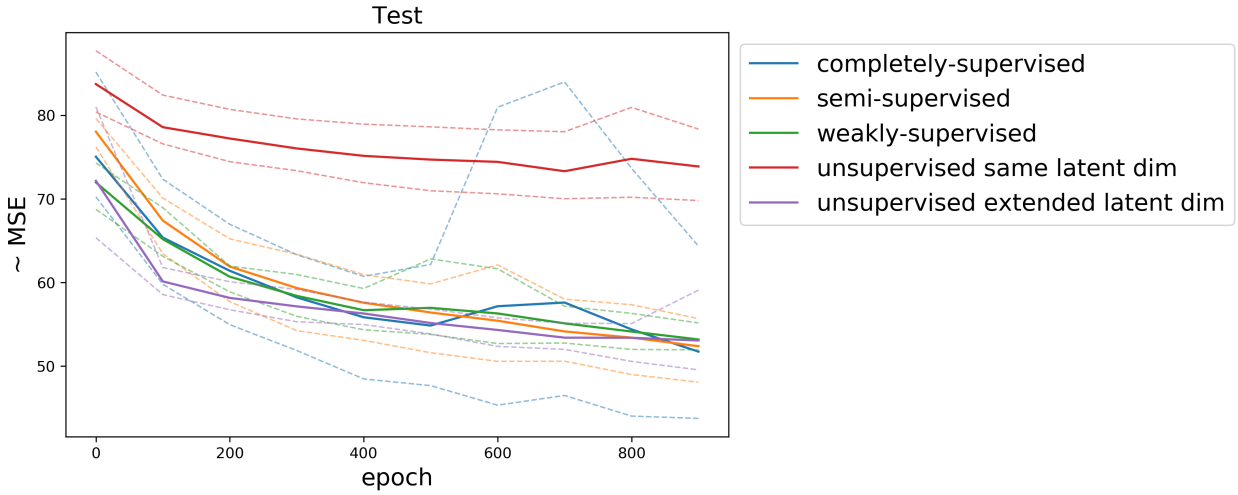

Figure 23: Comparison of different (semi-supervised) VAE models.

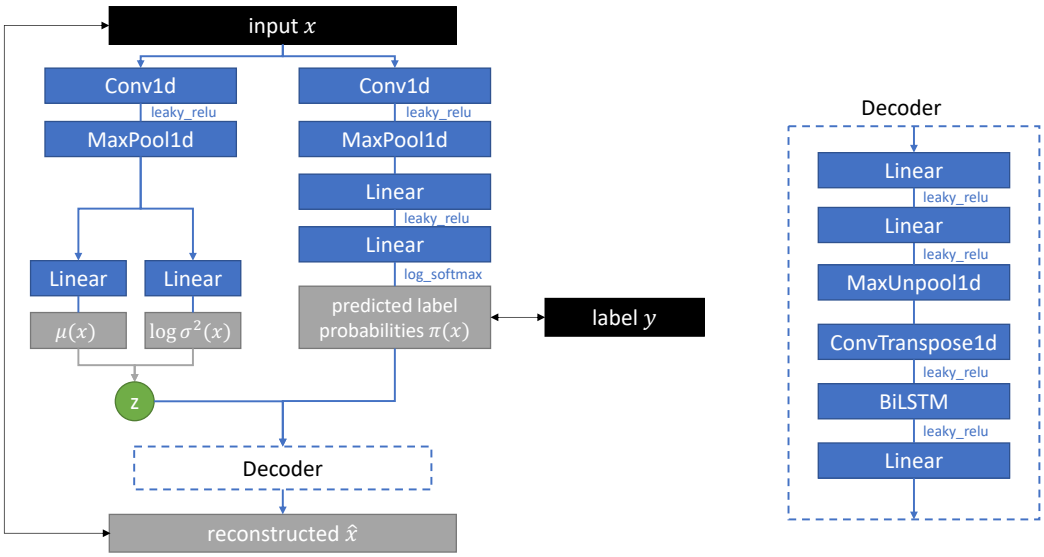

Figure 24: Semi-supervised VAE for time-series architecture.