

Unsupervised Anomaly Detection in Time Series Data using Deep Learning

Integrated Master in Electrical and Computer Engineering



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23rd November, 2018

Introduction & Motivation

Anomaly detection is about finding patterns in data that do not conform to *expected* or *normal* behaviour.



Main Challenges

- Most data in the world are **unlabelled**

$$\text{Dataset } \mathcal{D} = \left\{ \left(\mathbf{x}^{(i)}, \mathbf{y}^{*(i)} \right) \right\}_{i=1}^N \xrightarrow{\text{anomaly labels}}$$

- Annotating large datasets is difficult, time-consuming and expensive



- Time series have temporal structure/dependencies

$$\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_T) , \quad \mathbf{x}_t \in \mathbb{R}^{d_x}$$

Objectives

We would like:

- ▶ Unsupervised: no need for anomaly labels;
- ▶ Suitable for sequential data (e.g., time series);
- ▶ General;
- ▶ Scalable & efficient, allowing real-time detection.

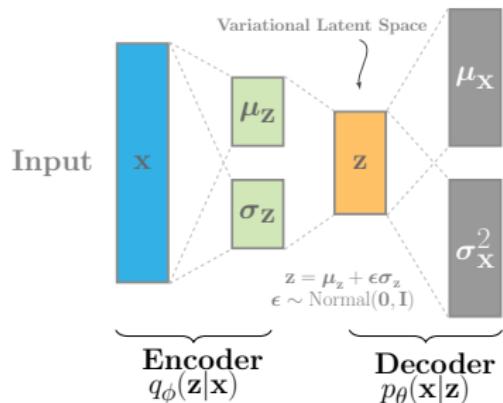
We would like:

- ▶ Unsupervised: no need for anomaly labels;
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- ▶ Scalable & efficient, allowing real-time detection.

How to design such a model?

The Principle in a Nutshell

- ▶ Train a **Variational Autoencoder**¹² to reconstruct input data with mostly normal patterns;



- ▶ At test time, it reconstructs well *normal* data, while it fails to reconstruct *anomalous* data;
- ▶ The quality of the reconstructions and the representations are used to compute anomaly scores.

¹Kingma & Welling, Auto-Encoding Variational Bayes, ICLR'14

²Rezende *et al.*, Stochastic Backpropagation and Approximate Inference in Deep Generative Models, ICML'14

Proposed Approach

Representation
Learning

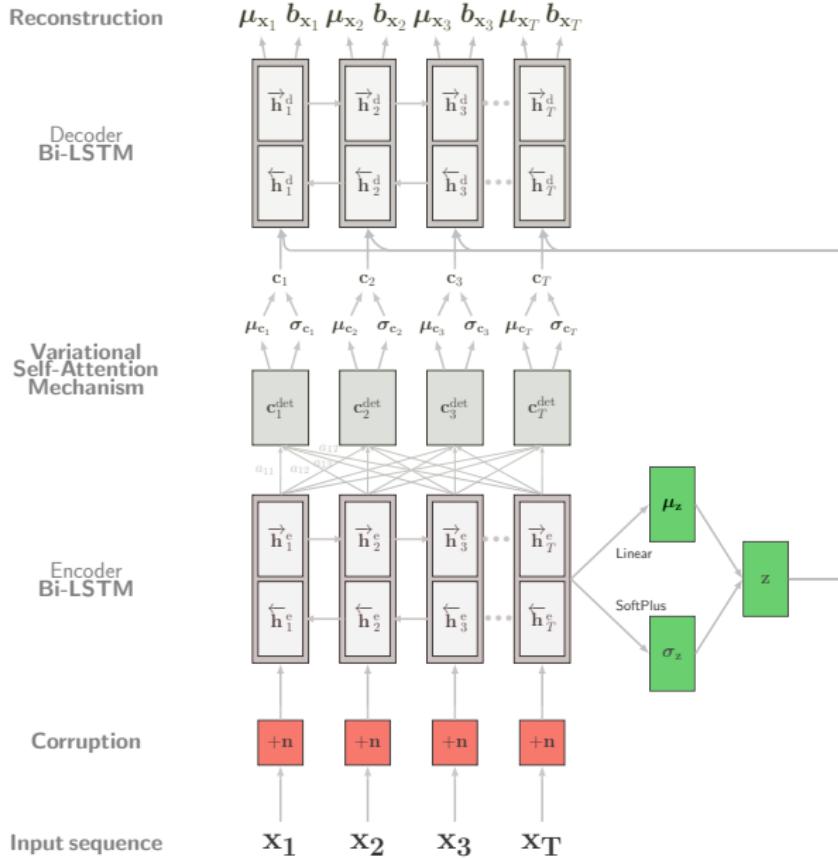
Detection

Proposed Approach

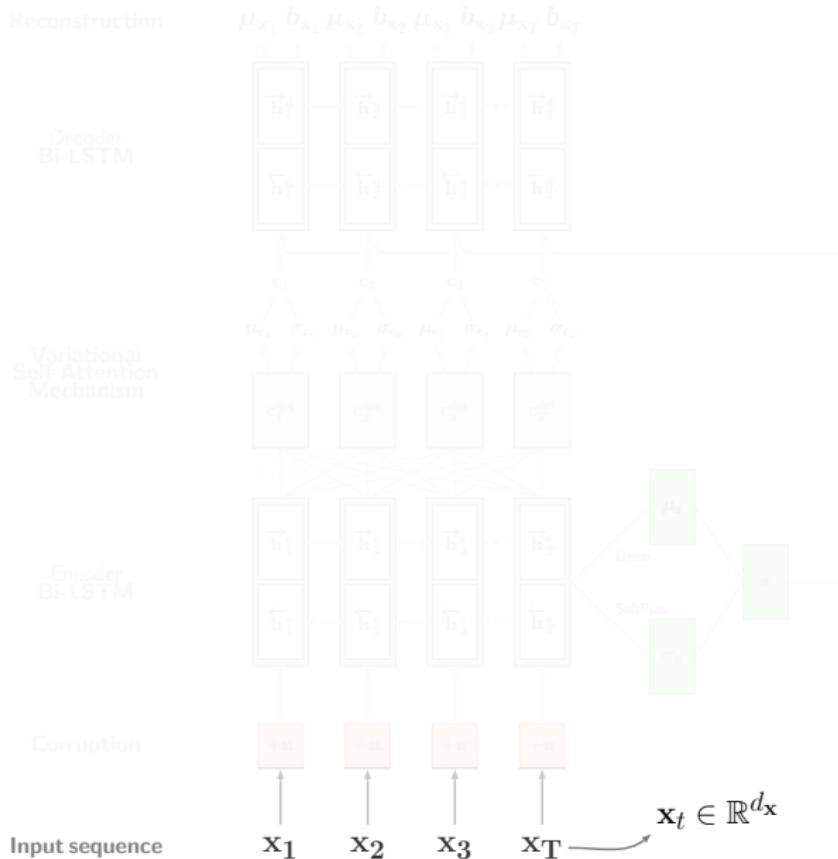
Representation
Learning

Detection

Representation Learning



Representation Learning



Representation Learning



Denoising Autoencoding Criterion

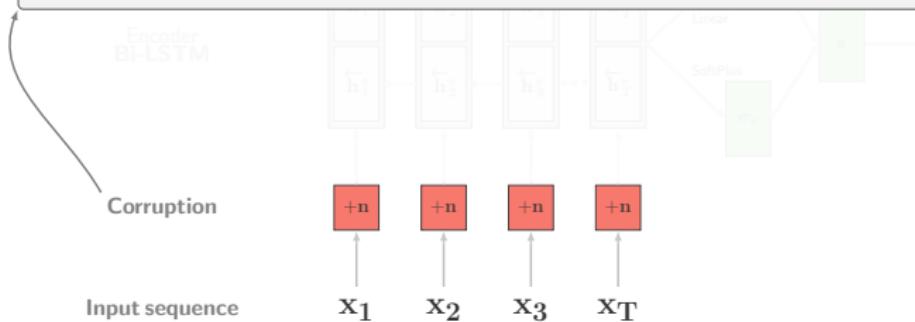
Corruption process: additive Gaussian noise

$$p(\tilde{x}|x) = x + n \quad , \quad n \sim \text{Normal}(0, \sigma_n^2 I)$$



Vincent *et al.*, Extracting and Composing Robust Features with Denoising Autoencoders, ICML'08

Bengio *et al.*, Denoising Criterion for Variational Auto-Encoding Framework, ICLR'15



Representation Learning

Learning temporal dependencies

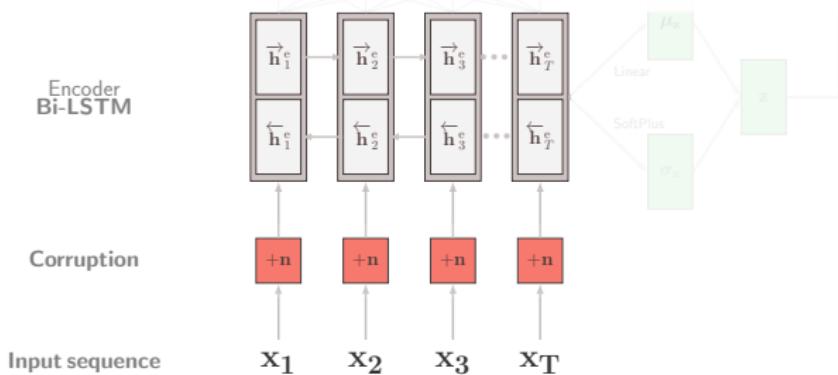
Bidirectional Long-Short Term Memory network

$$\mathbf{h}_t = [\vec{\mathbf{h}}_t; \overleftarrow{\mathbf{h}}_t]$$

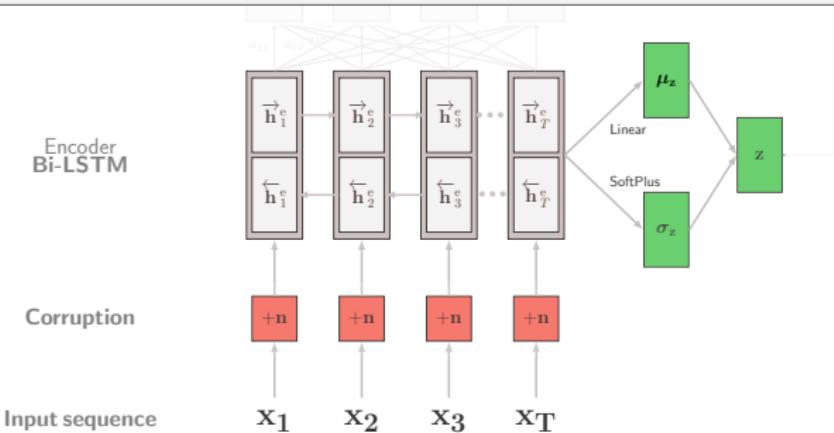
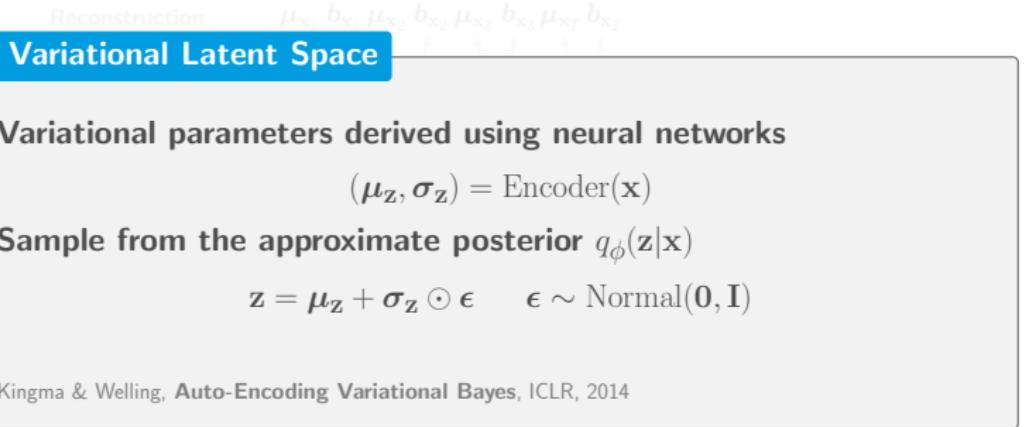
- ▶ 256 units, 128 in each direction
- ▶ Sparse regularization, $\Omega(\mathbf{z}) = \lambda \sum_{i=1}^{d_z} |z_i|$

Hochreiter *et al.*, Long-Short Term Memory, Neural Computation'97

Graves *et al.*, Bidirectional LSTM Networks for Improved Phoneme Classification and Recognition, ICANN'05



Representation Learning



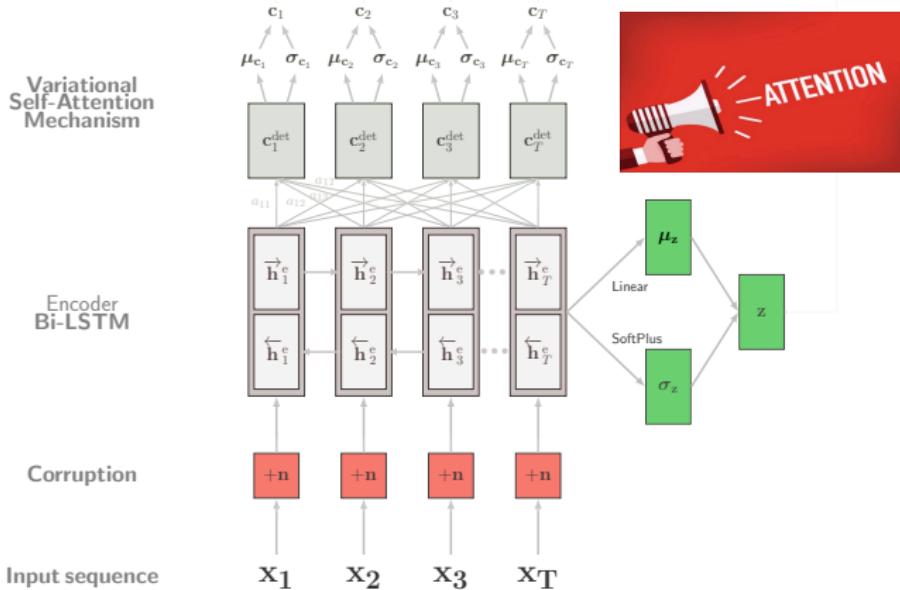
Representation Learning

Introducing Variational Self-Attention

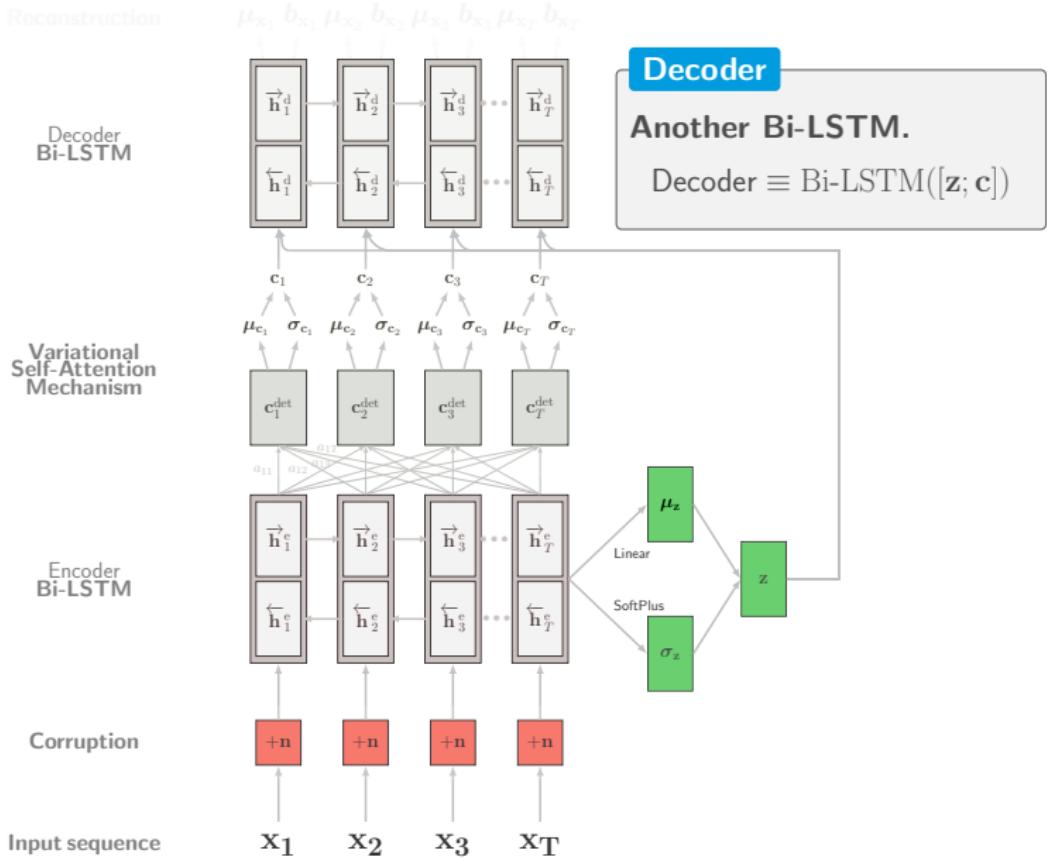
A combination of self-attention and variational inference.

$$\mathbf{c}_t^{\text{det}} = \sum_{j=1}^T a_{tj} \mathbf{h}_j \quad (\mu_{\mathbf{c}_t}, \sigma_{\mathbf{c}_t}) = \text{NN}(\mathbf{c}_t^{\text{det}}), \quad \mathbf{c}_t \sim \text{Normal}(\mu_{\mathbf{c}_t}, \sigma_{\mathbf{c}_t}^2 \mathbf{I})$$

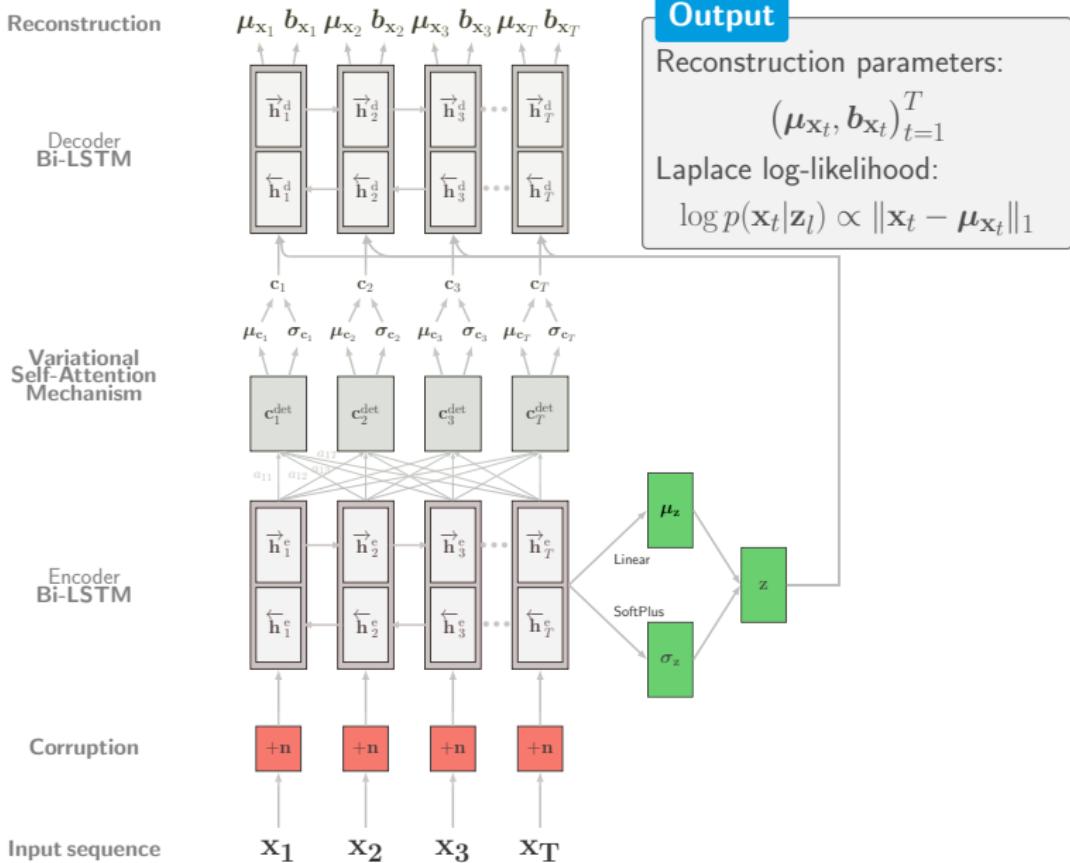
Vaswani et al., Attention is All You Need, NIPS'17



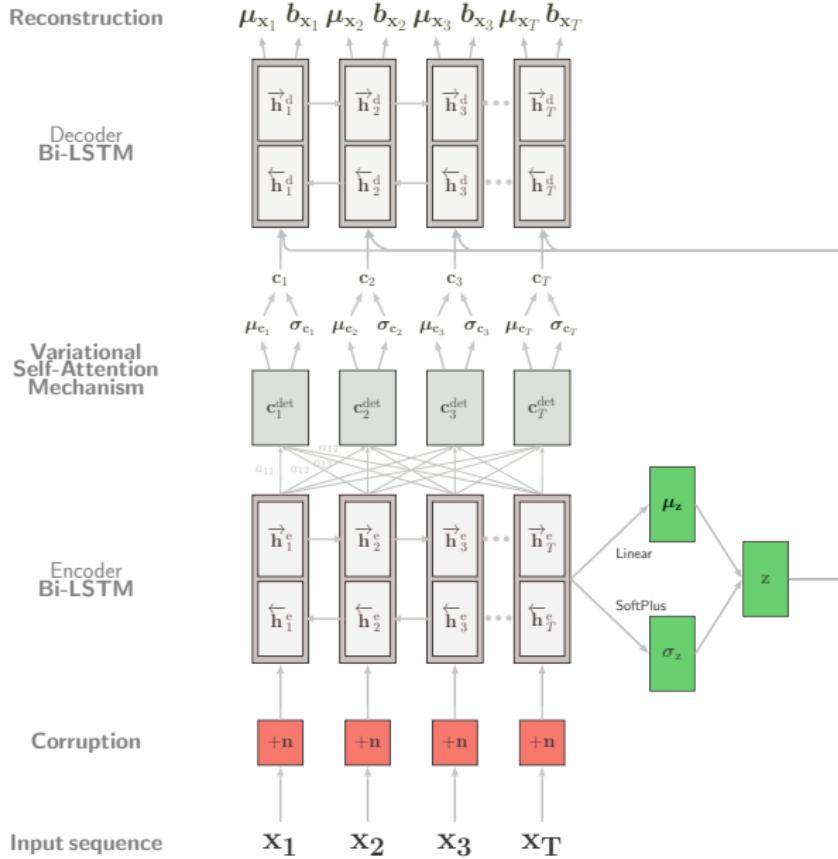
Representation Learning



Representation Learning



Representation Learning



Loss Function

Loss Function

$$\begin{aligned}\mathcal{L}(\theta, \phi; \mathbf{x}^{(n)}) &= -\mathbb{E}_{\mathbf{z} \sim \tilde{q}_\phi(\mathbf{z}|\mathbf{x}^{(n)}), \mathbf{c}_t \sim \tilde{q}_\phi^a(\mathbf{c}_t|\mathbf{x}^{(n)})} \left[\log p_\theta(\mathbf{x}^{(n)}|\mathbf{z}, \mathbf{c}) \right] \\ &+ \lambda_{\text{KL}} \left[\mathcal{D}_{\text{KL}} \left(\tilde{q}_\phi(\mathbf{z}|\mathbf{x}^{(n)}) \| p_\theta(\mathbf{z}) \right) + \eta \sum_{t=1}^T \mathcal{D}_{\text{KL}} \left(\tilde{q}_\phi^a(\mathbf{c}_t|\mathbf{x}^{(n)}) \| p_\theta(\mathbf{c}_t) \right) \right]\end{aligned}$$

\mathcal{D}_{KL} denotes the Kullback-Leibler Divergence

Loss Function

$$\begin{aligned}\mathcal{L}(\theta, \phi; \mathbf{x}^{(n)}) &= \overbrace{-\mathbb{E}_{\mathbf{z} \sim \tilde{q}_\phi(\mathbf{z}|\mathbf{x}^{(n)}), \mathbf{c}_t \sim \tilde{q}_\phi^a(\mathbf{c}_t|\mathbf{x}^{(n)})} \left[\log p_\theta(\mathbf{x}^{(n)}|\mathbf{z}, \mathbf{c}) \right]}^{\text{Reconstruction Term}} \\ &+ \lambda_{\text{KL}} \left[\underbrace{\mathcal{D}_{\text{KL}}\left(\tilde{q}_\phi(\mathbf{z}|\mathbf{x}^{(n)}) \| p_\theta(\mathbf{z})\right)}_{\text{Latent Space KL loss}} + \eta \sum_{t=1}^T \underbrace{\mathcal{D}_{\text{KL}}\left(\tilde{q}_\phi^a(\mathbf{c}_t|\mathbf{x}^{(n)}) \| p_\theta(\mathbf{c}_t)\right)}_{\text{Attention KL loss}} \right]\end{aligned}$$

\mathcal{D}_{KL} denotes the Kullback-Leibler Divergence

Optimization & Regularization

- ▶ About 270k parameters to optimize
- ▶ *AMS-Grad* optimizer³
- ▶ Xavier weight initialization⁴
- ▶ Denoising autoencoding criterion⁵
- ▶ Sparse regularization in the encoder Bi-LSTM⁶
- ▶ KL cost annealing⁷
- ▶ Gradient clipping⁸

Training executed on a single GPU (NVIDIA GTX 1080 TI)

³Reddi, Kale & Kumar, **On the Convergence of Adam and Beyond**, ICLR'18

⁴Bengio *et al.*, **Understanding the Difficulty of Training Deep Feedforward Neural Networks**, AISTATS'10

⁵Bengio *et al.*, **Denoising Criterion for Variational Auto-Encoding Framework**, AAAI'17

⁶Arpit *et al.*, **Why Regularized Auto-Encoders Learn Sparse Representation?**, ICML'16

⁷Bowman, Vinyals *et al.*, **Generating Sentences from a Continuous Space**, SIGNLL'16

⁸Bengio *et al.*, **On the Difficulty of Training Recurrent Neural Networks**, ICML'13

Proposed Approach

Representation
Learning

Detection

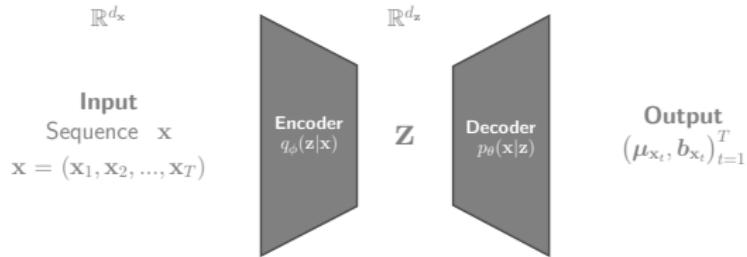
Proposed Approach

Representation
Learning

Detection

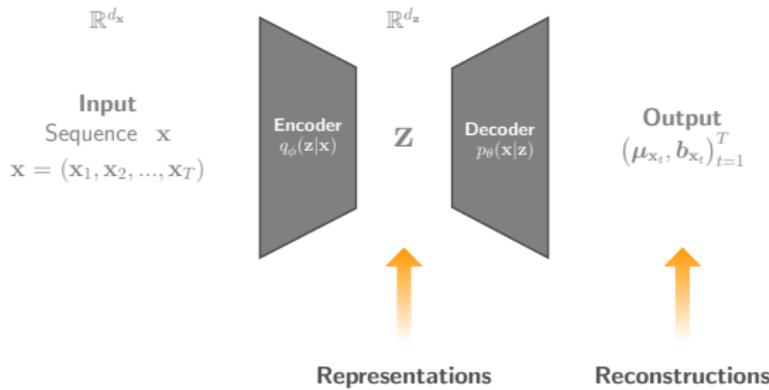
One model, two detection strategies

The model provides two products: **representations** in the z-space and the **reconstruction parameters** in the x-space



One model, two detection strategies

The model provides two products: **representations** in the z-space and the **reconstruction parameters** in the x-space



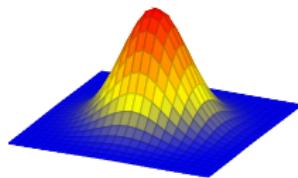
- ▶ Reconstruction-based detection
- ▶ Latent space-based detection

Reconstruction-based Detection

$$\text{Reconstruction Error} = \mathbb{E}_{\mathbf{z}_l \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[\|\mathbf{x} - \mathbb{E}[p_{\theta}(\mathbf{x}|\mathbf{z}_l)]\|_1 \right]$$

$$\text{Reconstruction Probability} = \mathbb{E}_{\mathbf{z}_l \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}_l) \right]$$

$$q_{\phi}(\mathbf{z}|\mathbf{x})$$

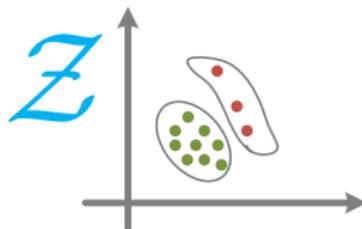


$$\mathbf{z}_l \sim \text{Normal}(\boldsymbol{\mu}_{\mathbf{z}}, \boldsymbol{\sigma}_{\mathbf{z}}^2 \mathbf{I})$$

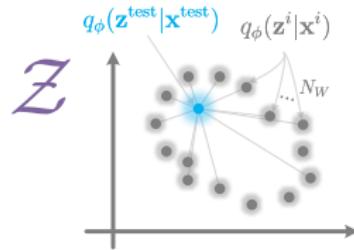
Latent Space Detection

Based on the representations in the z-space.

► Clustering



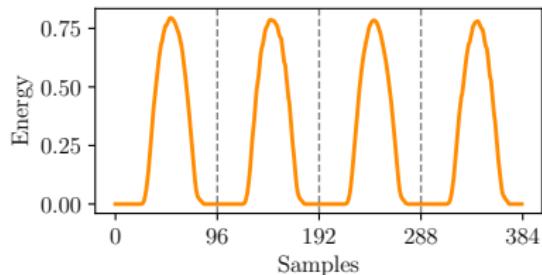
► Wasserstein Metric (W)



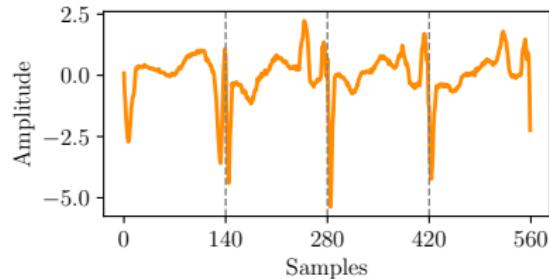
$$\text{score}(\mathbf{z}^{\text{test}}) = \text{median}\{W(\mathbf{z}^{\text{test}}, \mathbf{z}^i)^2\}_{i=1}^{N_W}$$

Time Series Data

Solar PV Generation



Electrocardiogram



- ▶ Provided by **c|side**
- ▶ Recorded every 15min (96 samples/day)
- ▶ Daily seasonality
- ▶ Unlabelled
- ▶ Available in the UCR Time Series Classification Archive ECG5000 [Keogh *et al.*, 2015]
- ▶ One heartbeat \approx 140 samples
- ▶ 5000 sequences
- ▶ Labelled, 5 classes annotated

Dataset

Energy



ECG5000



Dataset

Energy



ECG5000



Variational Latent Space

Energy

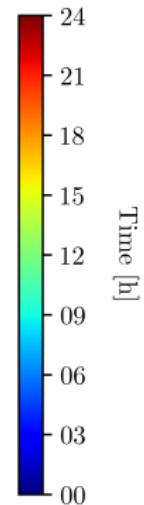
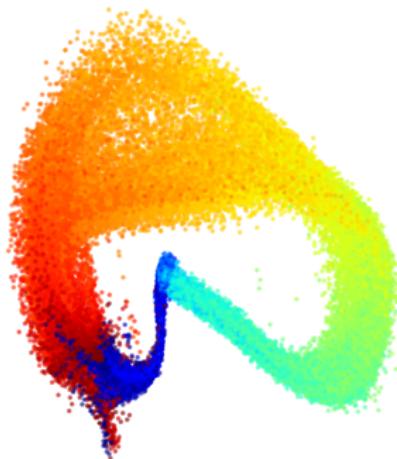
z-space in 2D ($\mathcal{X}_{\text{train}}^{\text{normal}}$)

$T = 12$ (< 96)
 $d_z = 3$
online mode

t-SNE

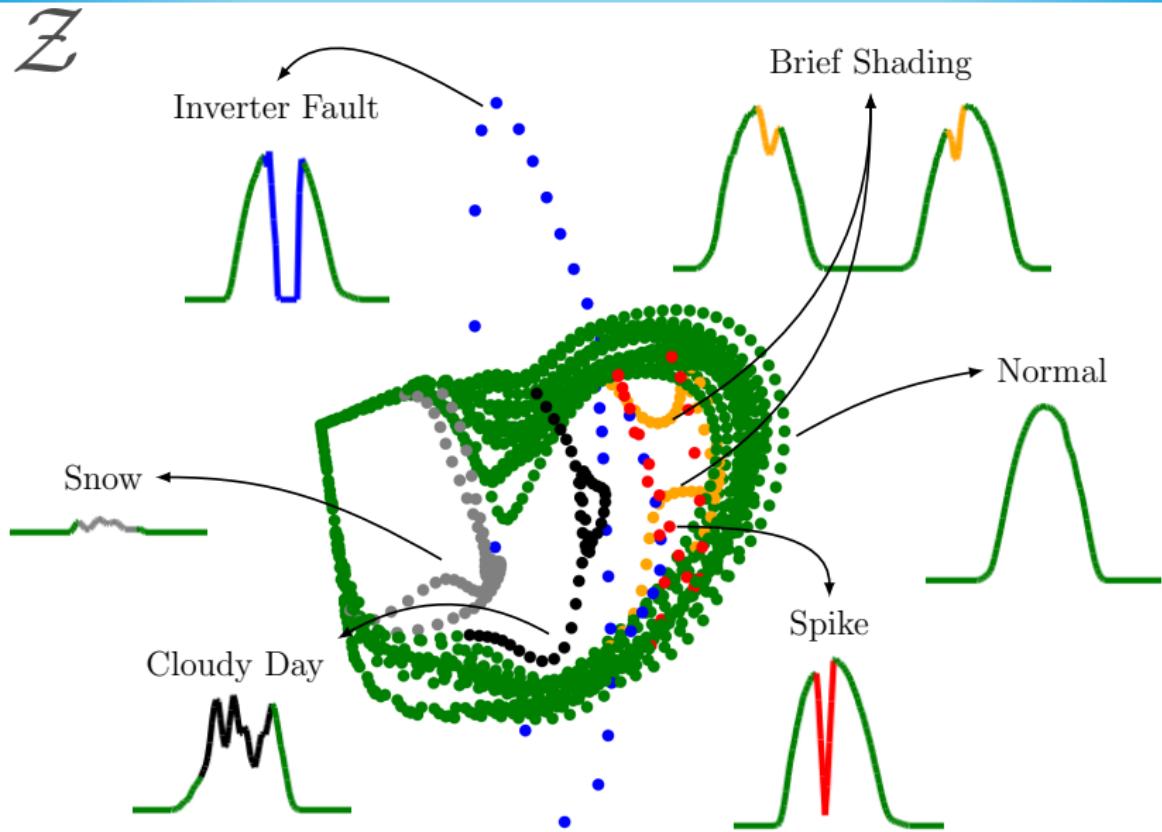


PCA

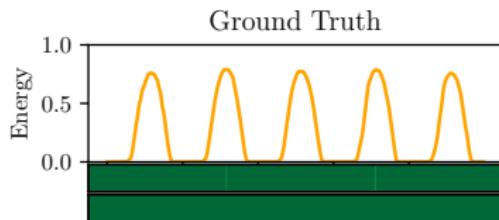


Finding Anomalies in the Latent Space

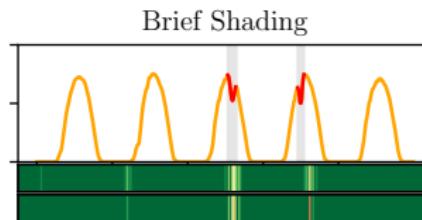
Energy



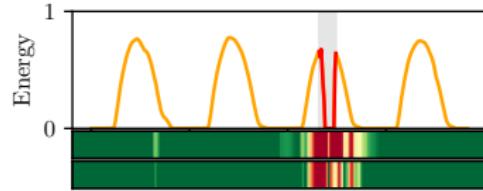
Reconstruction Error (top bar)



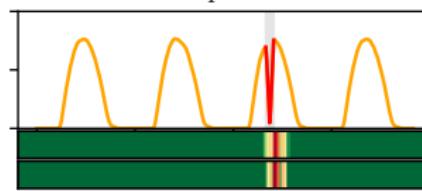
Reconstruction Probability (bottom bar)



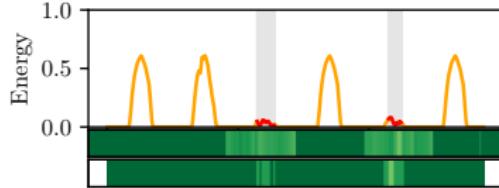
Inverter Fault



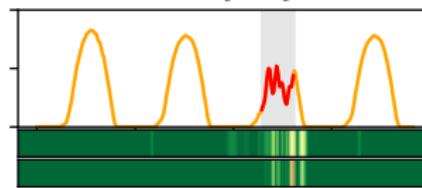
Spike



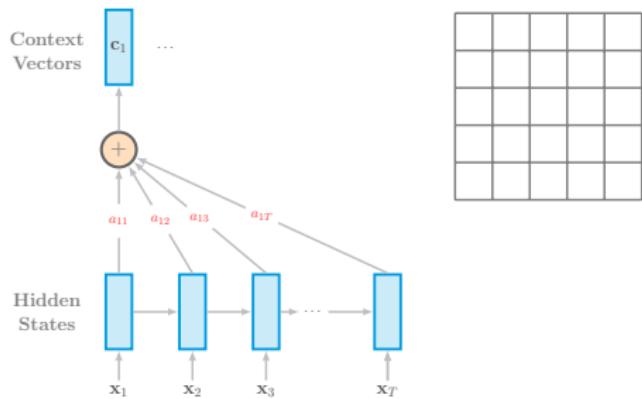
Snow



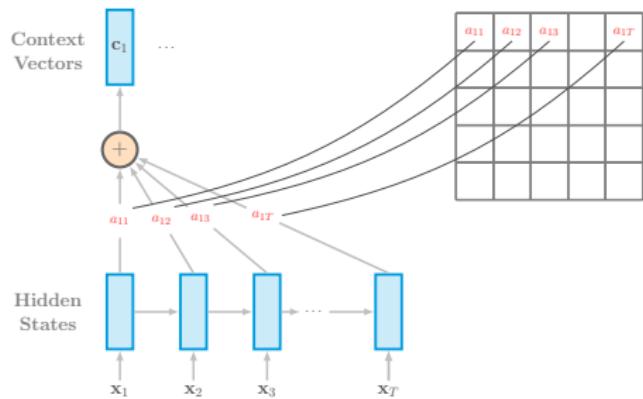
Cloudy Day



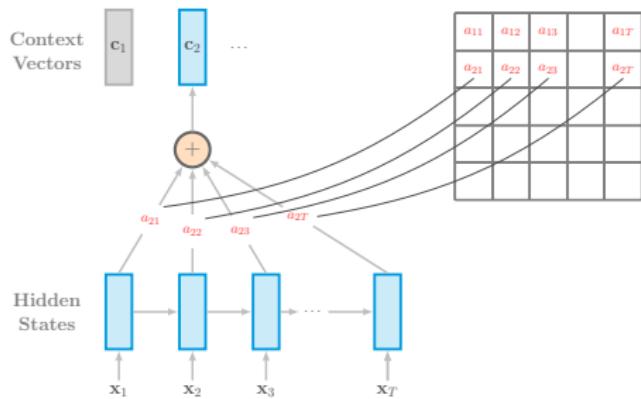
Attention Map



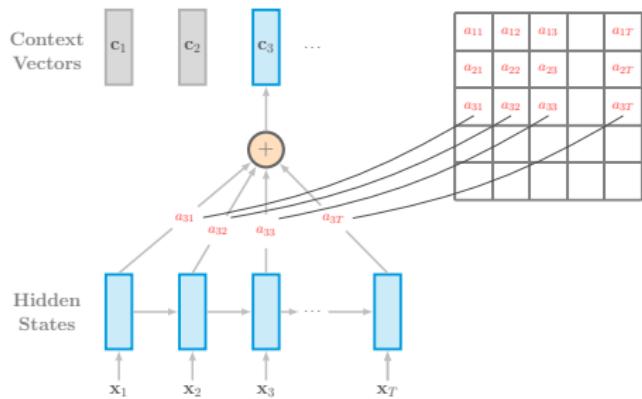
Attention Map



Attention Map

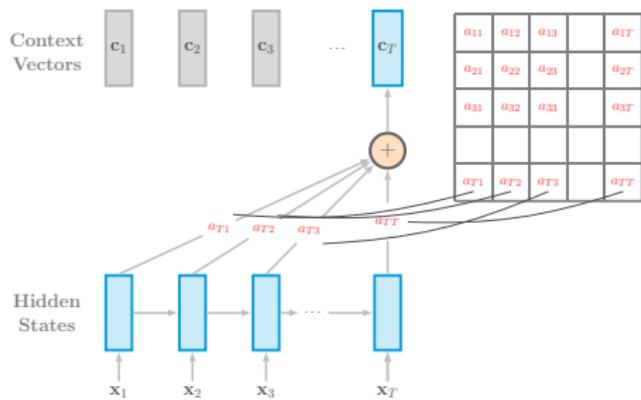


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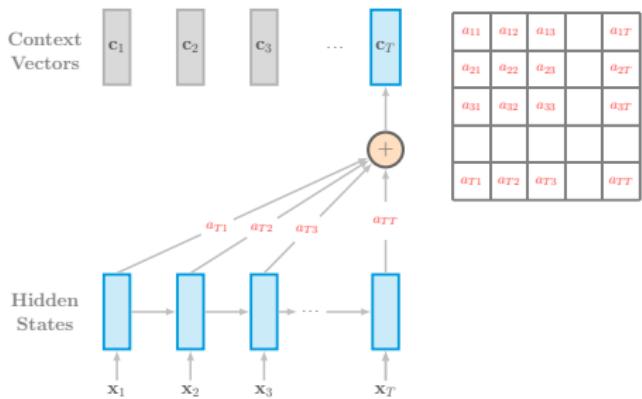


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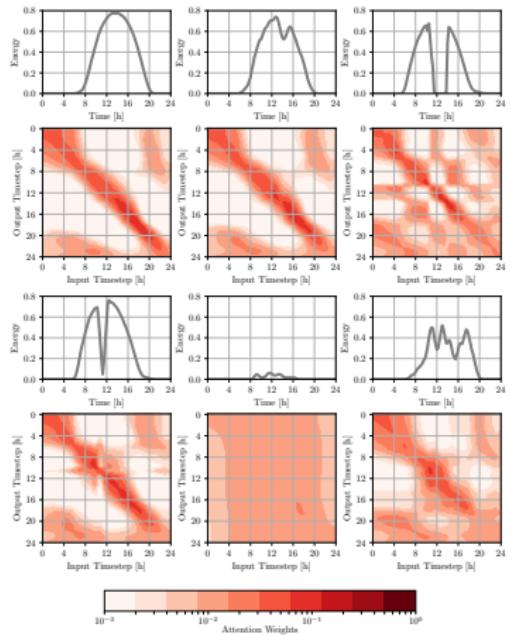
Examples



Attention Map



Examples



Dataset

Energy



ECG5000



Dataset

Energy

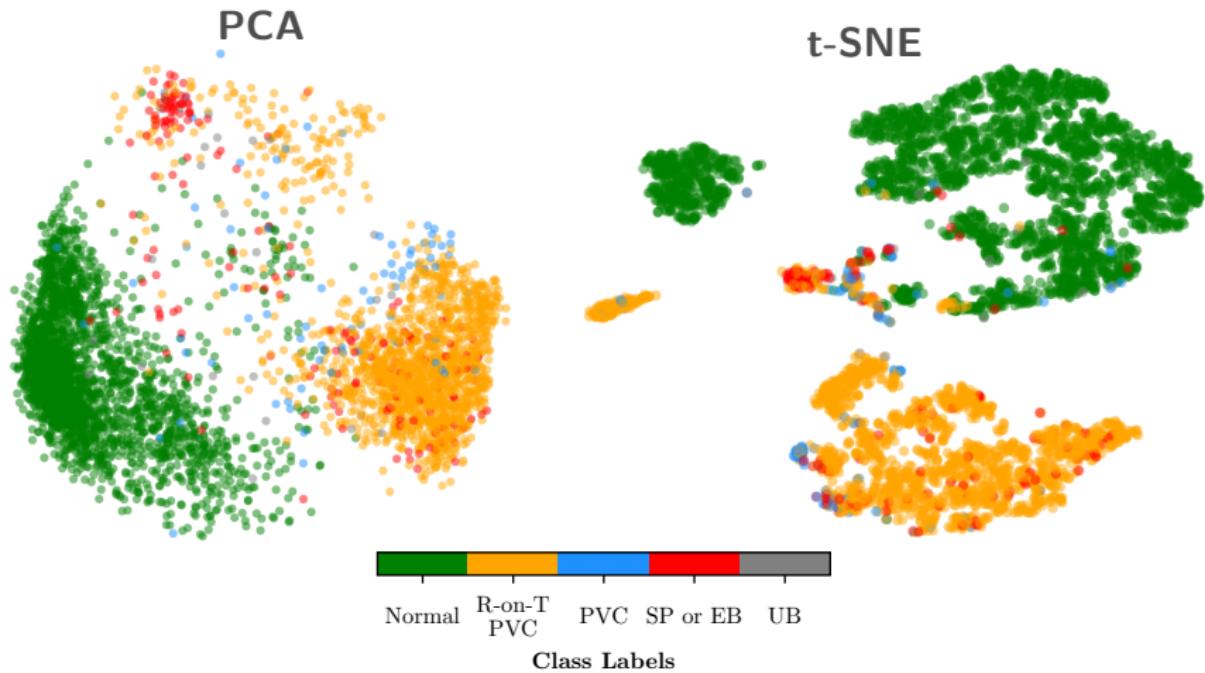


ECG5000



Each datapoint → a sequence of length T

$$\begin{aligned} T &= 140 \text{ (one heartbeat)} \\ d_z &= 5 \end{aligned}$$



Metric	Hierarchical	Spectral	<i>k</i> -Means++	Wasserstein	SVM
AUC	0.9569	0.9591	0.9591	0.9819	0.9836
Accuracy	0.9554	0.9581	0.9596	0.9510	0.9843
Precision	0.9585	0.9470	0.9544	0.9469	0.9847
Recall	0.9463	0.9516	0.9538	0.9465	0.9843
<i>F</i> ₁ -score	0.9465	0.9474	0.9522	0.9461	0.9844

Source	S/U	Model	AUC	Acc	<i>F</i> ₁
Proposed	S	VRAE+SVM	0.9836	0.9843	0.9844
	U	VRAE+Clust/W	0.9819	0.9596	0.9522
Lei <i>et al.</i> , 2017	S	SPIRAL-XGB	0.9100	-	-
Karim <i>et al.</i> , 2017	S	F-t ALSTM-FCN	-	0.9496	-
Malhotra <i>et al.</i> , 2017	S	SAE-C	-	0.9340	-
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Unsupervised

Supervised

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Conclusions & Future Work

The proposed approach is:

- ▶ Effective on detecting anomalies in time series data;
- ▶ Suitable for both **univariate and multivariate** data;
- ▶ **Efficient**: inference and anomaly scores computation is fast;
- ▶ Works with other kinds of sequential data (e.g., **text, videos**);
- ▶ Extensible to a **multi-class framework** that allows discrimination between anomalies.

Publications

Unsupervised Anomaly Detection in Energy Time Series Data using Variational Recurrent Autoencoders with Attention

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Abstract—In the age of big data, time series are being generated at massive amounts. In the energy field, smart grids are starting a transformational revolution with the integration of sensors and data collection. In this context, there has been an increasing interest in solar photovoltaic energy generation prediction and anomaly detection. These sensors measure the energy production. Such amount of data can be used to build smart systems that can detect anomalies in these systems, trigger alerts and prevent damage.

In this paper, we propose a generic, unsupervised and scalable framework for anomaly detection in time series data, based on a variational recurrent autoencoder. First, we introduce attention in the model, by means of a variational self-attention mechanism, which allows the model to focus on the encoding-decoding process. Afterwards, we perform anomaly detection in the latent space, which is created to take into account the order and structure of the data.

The main contribution of this work can be summarized in the following:

- Unsupervised reconstruction-based model using a variational autoencoder with recurrent encoder and decoder;
- Variational self-attention mechanism to improve the encoding-decoding process;
- Generic framework for anomaly detection in time series
- Application to solar photovoltaic generation time series.

II. BACKGROUND

In this section, we revise autoencoders, recurrent neural networks, attention mechanisms and autoencoder-based anomaly detection.

Accepted for Oral Presentation at the
17th IEEE International Conference on
Machine Learning and Applications

Learning Representations from Healthcare Time Series Data for Unsupervised Anomaly Detection

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Abstract—The amount of raw data generated in healthcare is growing very fast and so is the need for methods that can analyse these data, detect anomalies and provide meaningful insights. In this context, there has been an increasing interest in anomaly detection in the streams. Therefore, anomaly detection in the streams has been a great challenge for researchers and practitioners.

However, most of the existing learning with deep generative models has been applied to flat representations of data, such as images and text. Motivated by this lack of approaches to streams, we propose an unsupervised framework for anomaly detection in time series data. This framework is based on representation learning using a Variational Recurrent Autoencoder. Afterwards, based on these representations, we define a distance metric to detect anomalies in the time series.

The main contribution of this work can be summarized as:

- Unsupervised representation learning of time series data through a Variational Recurrent Autoencoder;
- Latent space-based detection using Clustering and the Wasserstein distance.

I. INTRODUCTION

In this work, we propose an unsupervised framework for anomaly detection in sequential data, based on representation learning using a Variational Recurrent Autoencoder and anomaly detection in the representation space via Clustering and Wasserstein distance.

This paper is organized as follows. We start by revising Autoencoders, Variational Autoencoders and Recurrent Neural Networks. After that, we propose our proposed approach to anomaly detection in time series data. Afterwards, we introduce our proposed representation learning model and its main metrics. Finally, we present and analyse the results obtained with our model in three datasets (ECG) time series.

Our contributions in this work can be summarized as:

- Unsupervised representation learning of time series data through a Variational Recurrent Autoencoder;
- Latent space-based detection using Clustering and the Wasserstein distance.

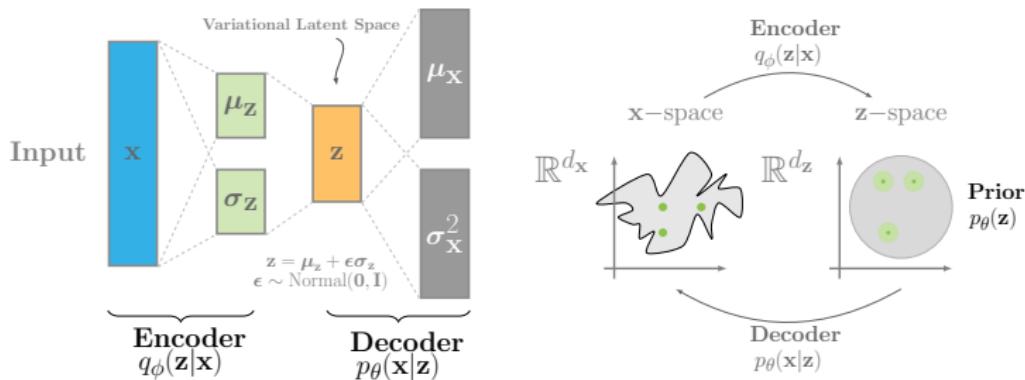
II. BACKGROUND

In this section, we revise Autoencoders, Variational Autoencoders and Recurrent Neural Networks, including Long Short-Term Memory Networks.

Thank you for your attention!

The Variational Autoencoder

- Deep generative model rooted in Bayesian inference



$$p_\theta(\mathbf{x}) = \int_{\mathbf{z}} p_\theta(\mathbf{z}) p_\theta(\mathbf{x}|\mathbf{z}) d\mathbf{z} \quad p_\theta(\mathbf{z}|\mathbf{x}) = \frac{p_\theta(\mathbf{z}) p_\theta(\mathbf{x}|\mathbf{z})}{p_\theta(\mathbf{x})}$$

- **Objective:** Maximize the Evidence Lower Bound (ELBO)

$$\log p_\theta(\mathbf{x}) \geq \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\log p_\theta(\mathbf{x}|\mathbf{z})] - \mathcal{D}_{\text{KL}}(q_\phi(\mathbf{z}|\mathbf{x}) \| p_\theta(\mathbf{z}))}_{:= \mathcal{L}_{\text{ELBO}}(\theta, \phi; \mathbf{x})}$$

Kingma & Welling, **Auto-Encoding Variational Bayes**, ICLR'14

Rezende et al., **Stochastic Backpropagation and Approximate Inference in Deep Generative Models**, ICML'14

Derivation of the Evidence Lower Bound (ELBO)

$$\begin{aligned}\log p_\theta(\mathbf{x}) &= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\log p_\theta(\mathbf{x})] \\&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})}{p_\theta(\mathbf{z}|\mathbf{x})} \right] \\&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})}{p_\theta(\mathbf{z}|\mathbf{x})} \frac{q_\phi(\mathbf{z}|\mathbf{x})}{q_\phi(\mathbf{z}|\mathbf{x})} \right] \\&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\log p_\theta(\mathbf{x}|\mathbf{z})] - \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \left[\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z})} \right] + \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \left[\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z}|\mathbf{x})} \right] \\&= \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\log p_\theta(\mathbf{x}|\mathbf{z})]}_{=\mathcal{L}_{\text{ELBO}}(\theta, \phi; \mathbf{x})} - \mathcal{D}_{\text{KL}}(q_\phi(\mathbf{z}|\mathbf{x}) \| p_\theta(\mathbf{z})) + \underbrace{\mathcal{D}_{\text{KL}}(q_\phi(\mathbf{z}|\mathbf{x}) \| p_\theta(\mathbf{z}|\mathbf{x}))}_{\geq 0}\end{aligned}$$

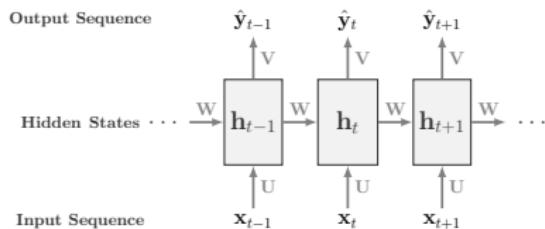
Recurrent Neural Networks

What if data are not i.i.d. in time?

(e.g., time series, text, videos)

RNNs capture the temporal dependencies of the data

- ▶ Real-valued hidden state \mathbf{h}_t
- ▶ Feedback connection
- ▶ Parameters shared across timesteps



$$\mathbf{h}_t = f(\mathbf{U}\mathbf{x}_t + \mathbf{W}\mathbf{h}_{t-1})$$

f is typically a tanh or sigmoid

Long Short-Term Memory Network

- ▶ Proposed to solve the vanishing gradient problem
- ▶ New cell and three gates
- ▶ Updates:

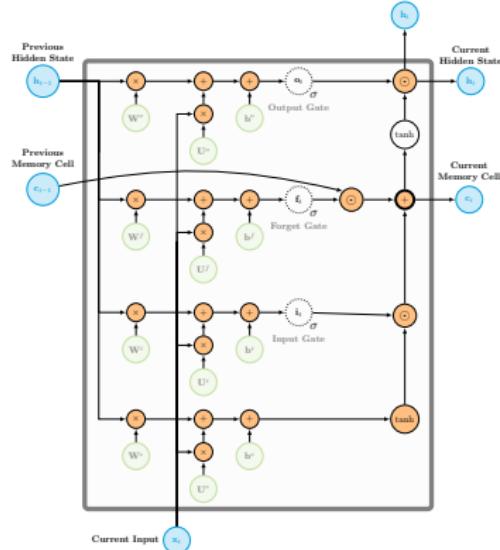
$$\mathbf{i}_t = \sigma(\mathbf{W}_i \mathbf{h}_{t-1} + \mathbf{U}_i \mathbf{x}_t + \mathbf{b}_i)$$

$$\mathbf{f}_t = \sigma(\mathbf{W}_f \mathbf{h}_{t-1} + \mathbf{U}_f \mathbf{x}_t + \mathbf{b}_f)$$

$$\mathbf{o}_t = \sigma(\mathbf{W}_o \mathbf{h}_{t-1} + \mathbf{U}_o \mathbf{x}_t + \mathbf{b}_o)$$

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tanh(\mathbf{W}_c \mathbf{h}_{t-1} + \mathbf{U}_c \mathbf{x}_t + \mathbf{b}_c)$$

$$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{c}_t)$$

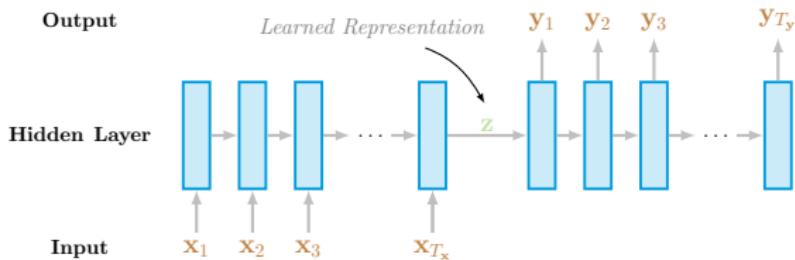


Hochreiter *et al.*, Long-Short Term Memory, Neural Computation'97

Graves *et al.*, Bidirectional LSTM Networks for Improved Phoneme Classification and Recognition, ICANN'05

Sequence to Sequence (Seq2Seq) models

Map sequences to sequences is useful.



Sutskever *et al.*, Sequence to Sequence Learning with Neural Networks, NIPS'14

Cho *et al.*, Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation, NIPS'14

Classification Metrics

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + FN + TN}$$

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

$$F_1\text{-score} = 2 \frac{\text{Precision} * \text{Recall}}{\text{Precision} + \text{Recall}}$$

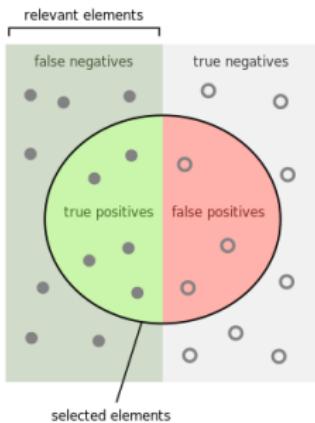
Legend:

TP : True Positives

TN : True Negatives

FP : False Positives

FN : False Negatives



How many selected items are relevant?

$$\text{Precision} = \frac{\text{green}}{\text{red + green}}$$

How many relevant items are selected?

$$\text{Recall} = \frac{\text{green}}{\text{green + black}}$$

Classification Metrics

AUC: Area under the Receiver Operating Characteristic Curve
(average precision over recalls)

