### Introduction

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Date:

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Paul O'Leary 6. July 2022

CoA2022-MLSC

Lecture

#### Chair of Automation

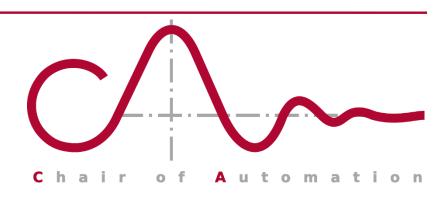
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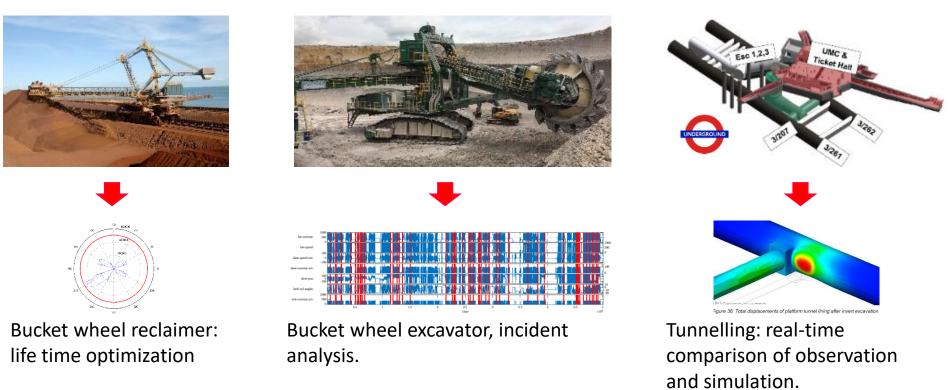


### Digitalization and CPS at the Chair of Automation

#### Recent and current projects



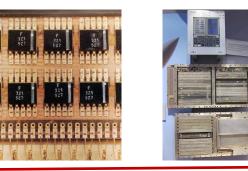
#### Three selected examples



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### 50 Years of Computing Technology



### Apollo Guidance Computer

2,800 ICs

36 K-words memory (16 Bit)

11.72 micro-seconds, (approx. 100 KHz).

16. July 1969



#### Nexus

CPU: Octa-core, 1.5GHz

GPU: Adreno 430

128 GB Memory

Comparison:

1.000.000 times more computing power

2.000.000 times more memory, etc. etc.

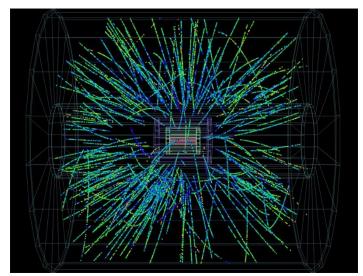
## It's not a question of technology It's what we do with the technology



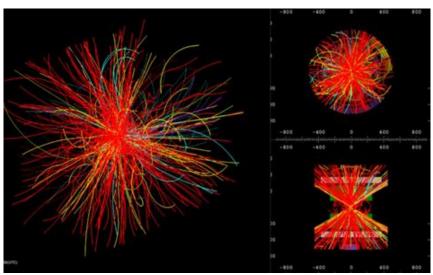


### Large Hadron Collider





Atlas



Alice

7/6/2022 Paul.oleary@unileoben.ac.at



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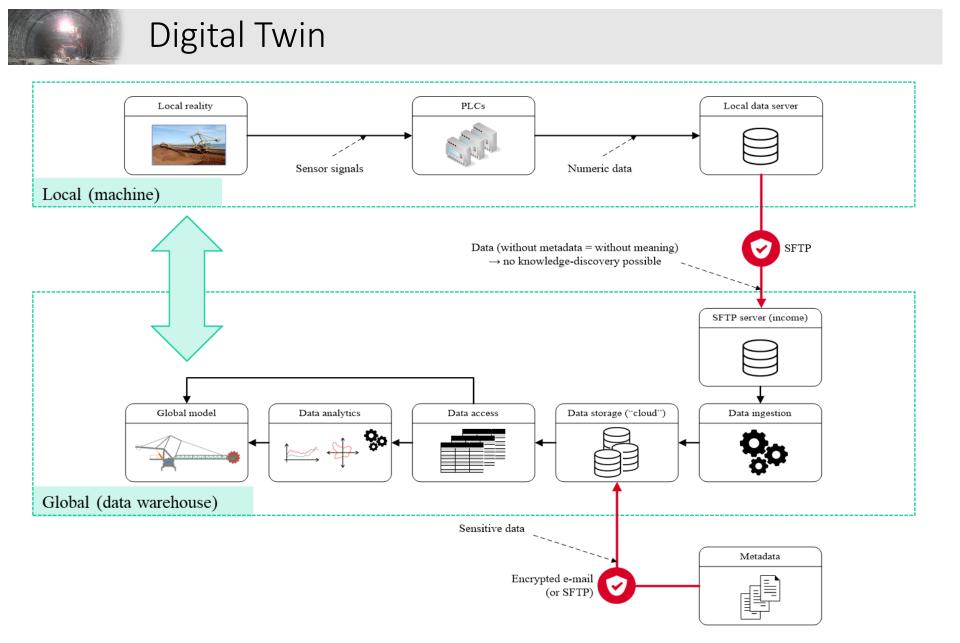


The most succinct and pertinent definition of a cyber physical system is:

"A CPS is a system with a coupling of the cyber aspects of computing and communications with the physical aspects of dynamics and engineering **that must abide by the laws of physics**. This includes sensor networks, real-time and hybrid systems."

Consequently:

- Mere correlation in the sensor data is an inadequate measure of significance.
- System models and their inverse solutions are required if sensor data analytics is to infer knowledge with respect to causality.
   System Identification, Embedded Simulation, Inverse problem to identify cause.
- No causality  $\rightarrow$  No semantics. No semantics  $\rightarrow$  No knowledge.





### **Economic Justification**

Incident analysis

Given an incident with the plant or machinery we can investigate the cause. This is important for both liability and guarantee reasons. Financially this has proved to be one of the most important issues.

• Commissioning support:

shortening the time to start up complex plant and machinery

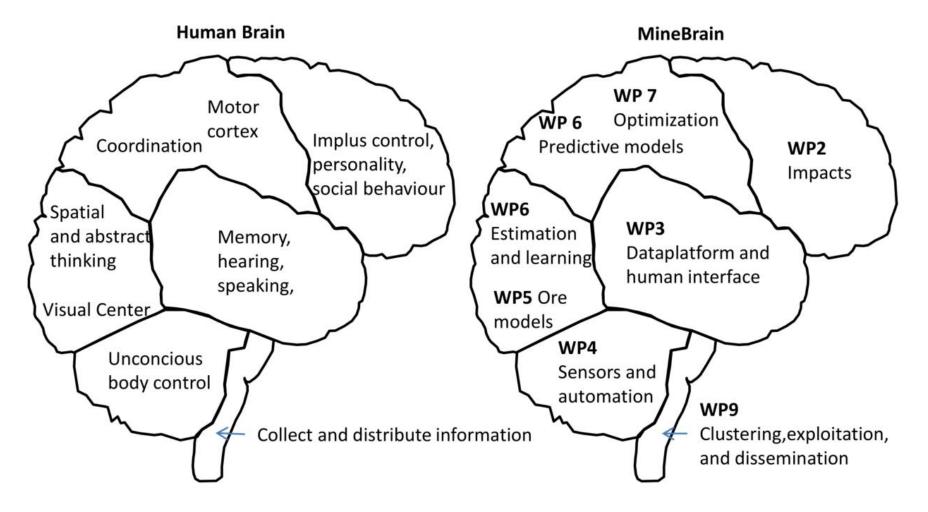
- Automatic operations recognition:
   Identifying incorrect operation, comparison of operation performance between operators
- Operational efficiency optimization:
   Finding invisible lost time
- Logistics optimization
   The logistics have an effect on machine life-times
- Fleet management
   Comparing the performance of multiple pieces of equipment
- Plant condition monitoring
   System identification to determine changes in system behaviour
- Material condition monitoring
   With established models effects of material condition can be separated from machine condition
- Engineering feedback

Possible improvements in machine design can be identified, important for the next generation.



### Intelligence and Artificial Intelligence

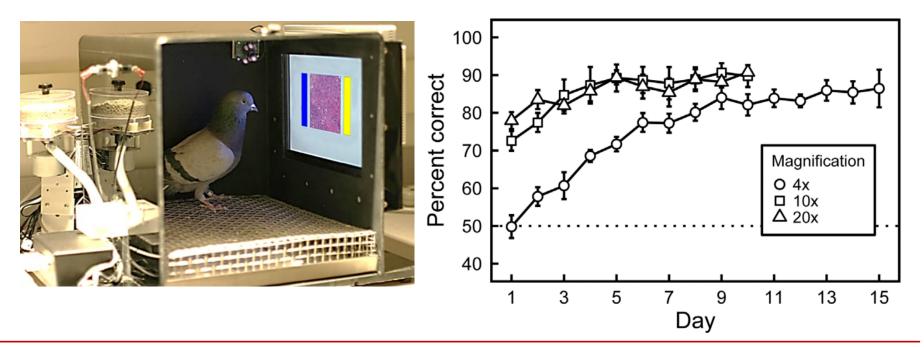
### Proposal for the "Mine Brain" project



## Perception and Understanding

### Pigeons (*Columba livia*) as Trainable Observers of Pathology and Radiology Breast Cancer Images

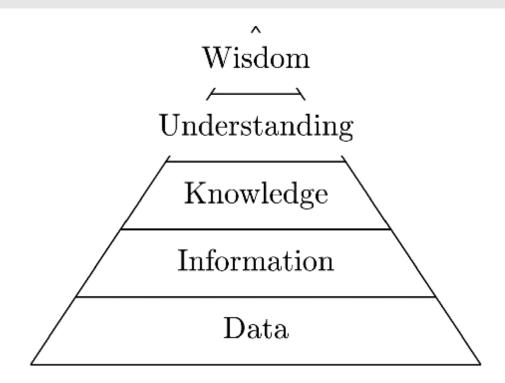
Richard M. Levenson<sup>1</sup>\*, Elizabeth A. Krupinski<sup>3</sup>, Victor M. Navarro<sup>2</sup>, Edward A. Wasserman<sup>2</sup>\*



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### What exists and what do we know?



### Ontology

What exists and which relationships are there?

### Epistemology

What do we know? how do we know it? And what are the limitations of knowing?



### A fundamental question

"What is a valid source of knowledge?"

Some ensuing questions:

- What is belief?
- What is justified belief and what justifies justified?
- What is the difference between justified belief, knowledge and understanding?
- How do we know that we know?





"What is a valid source of knowledge?"

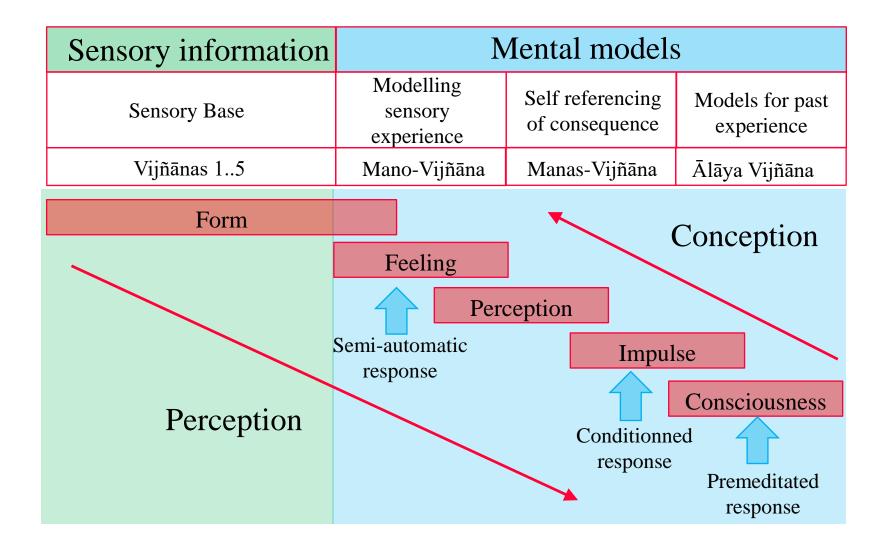
European Phenomonology as a possible answer:

- Edmund Husserl (April 8, 1859 April 27, 1938)
   "... experience is the source of all knowledge..."
  - Martin Heidegger (September 26, 1889 May 26, 1976) "... the things in lived experience always have more to them than what we can see...".

(Hidden models)

Maurice Merleau-Ponty (14 March 1908 – 3 May 1961)
 "...first we experience and then we reflect...."







### Galileo Galilei

#### (15. Feb. 1564 - 29. Dec. 1641)

### **Observational science**

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Born in 1564, Galileo Galilei's observations of our solar system and the Milky Way revolutionized the understanding the Universe.

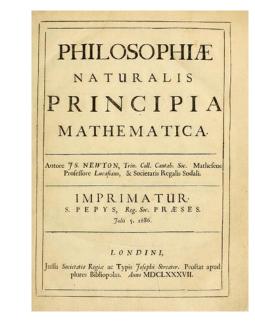
Draft of a letter to Leonardo Donato, Doge of Venice, August, 1609, and Notes on the Moons of Jupiter, January 1610. Credit: University of Michigan Special Collections Library



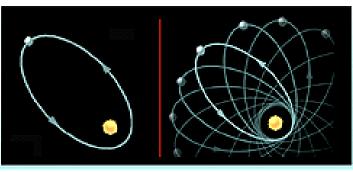
Isaac Newton

### Mathematical models of observation (Physical laws)





#### MERCURY'S ORBIT

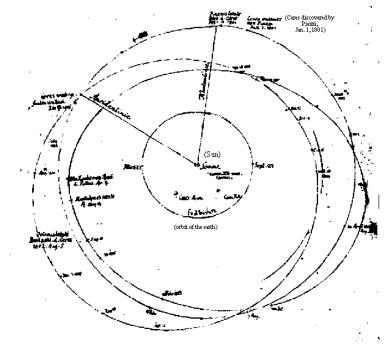


 $F_g = G \frac{m_1 m_2}{r^2}$ 



### Mathematical science of systems and uncertainty





Sketch of the orbits of Ceres and Pallas (nachlaß Gauß, Handb. 4). Courtesy of Universitätsbibliothek Göttingen.

# Gauss developed the statistical methods of least squares to determine the orbit of Ceres, which was first observed by Galilei.

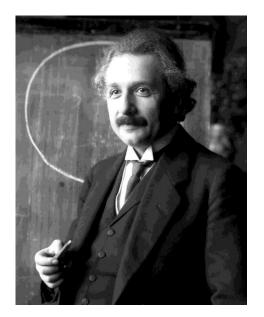
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Albert Einstein

(14. Mar. 1879 - 18. Apr. 1955)

### Connectional paradigm change emerging from abstract thinking



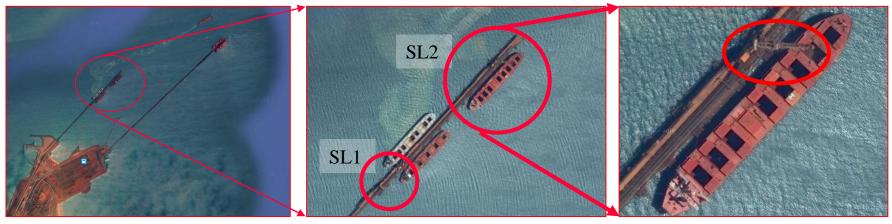
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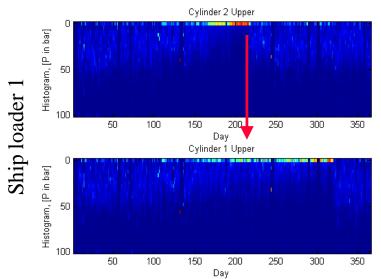
$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} = \frac{8 \pi G}{c^4} T_{\mu\nu}$$

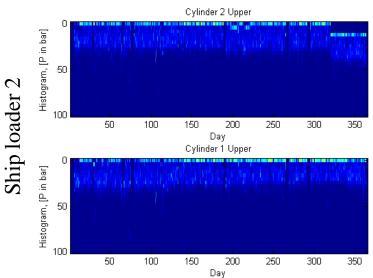
# A relationship between gravity and **time**-space.

#### Cape Lambert: an Exemplary Case



One year of operating data for the hydraulics of the two ship loaders

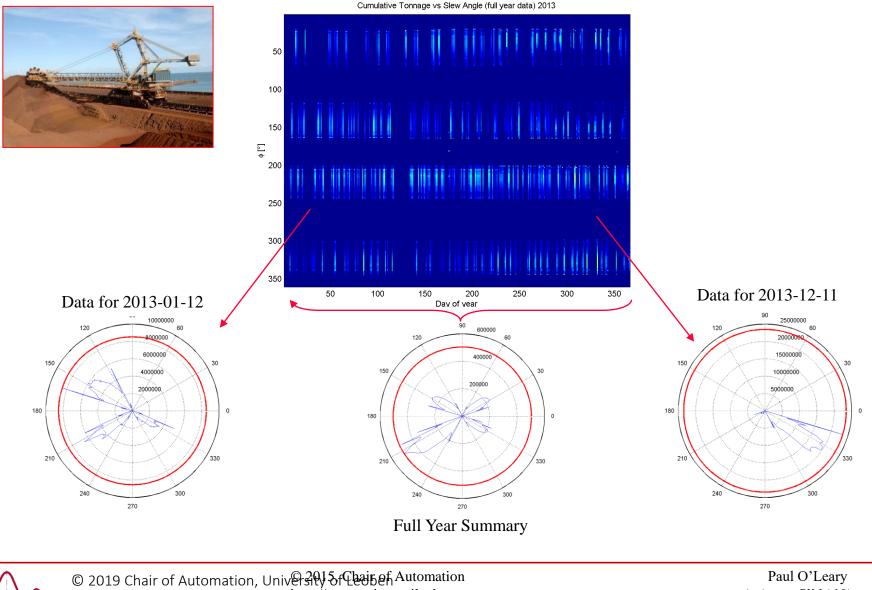




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#### From a Years Overview to Slew-Bearing Loading on a Specific Day



http://automation.unileoben.ac.at

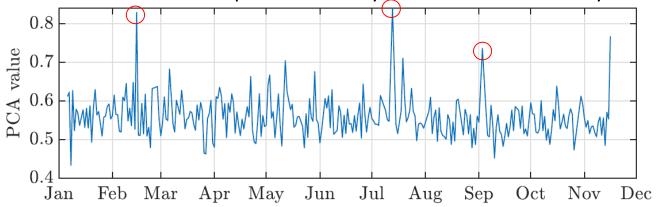
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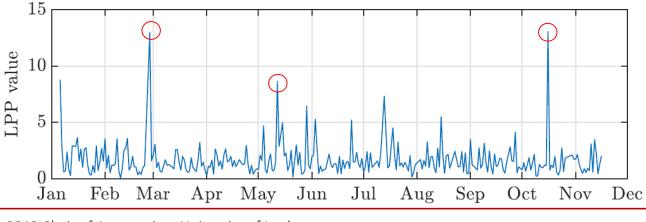


D4.2.3: Example – PCA and LPP

- For the data on the server.
- PCA and LPP were performed to the array of summary tables.
- PCA can be used to represent days of lower activity.



LPP can be used to represent significant changes in the data.



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### D4.3.1: Visualization of CCA results

January									
			1	2	3	4			
5	6	7	8	9	10	11			
2	13	14	15	16	17	18			
9	20	21	22	23	24	25			
6	27	28	29	30	31				

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19	20	21	22	23	24
26	27	28	29	30	31
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28	29	30				

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#### February

Year = 2014

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23	24	25	26	27	28	

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**13 14 15 16** 17 18 **19** 21 22 23 24 25 26

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November

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16 17 18 19 20 21 22 23 24 25 26 27 28 29

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28 29 30 31

12

6 7

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30

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27	28	29	30			
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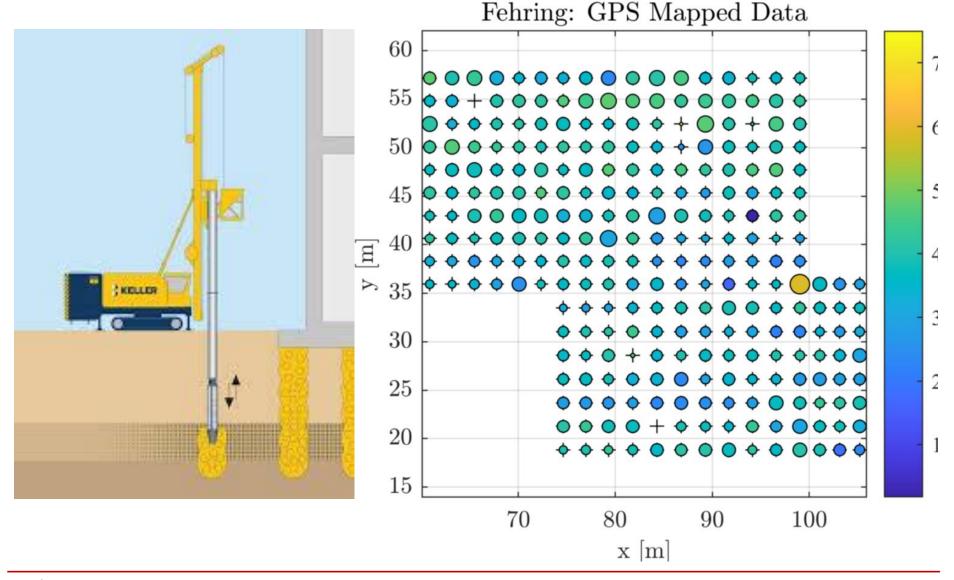
December						
<u> </u>	1	2	3	4	5	6
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14	15	16	17	18	19	20
21	22	23	24	25	26	$27 \cdot$
28	29	30	31			
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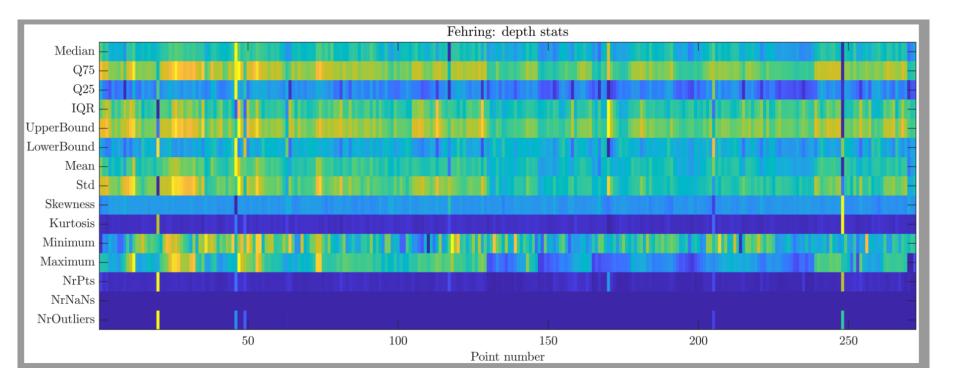
### Location Mapped Data



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### Anomaly Heat Maps





The Universe

- 5% "normal matter", i.e., the rest everything on Earth, everything ever observed, everything we claim to know anything about!
- 27%. dark matter.
- 68% dark energy.

Abell 520: observation seems to indicate the current theories of dark matter are not correct.



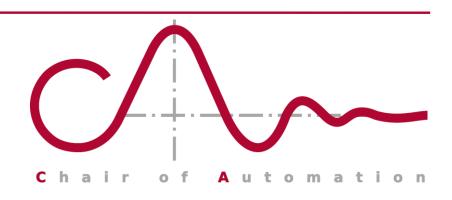
## Hybrid Machine Learning for Anomaly Detection in Industrial Time-Series Measurement Data

Authors:	Anika Terbuch, Paul OʻLeary, Peter Auer
Presenter:	Paul O'Leary
Date:	6 July 2022
Conference:	Summer School – Data Science hub

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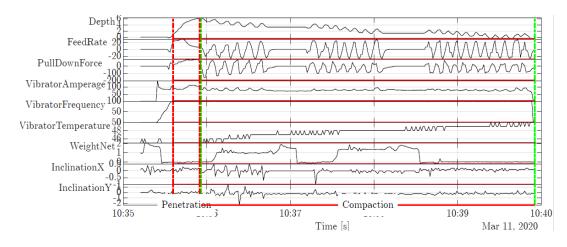
Motivation

- Improving the detection of anomalies in multivariate time-series (MVTS)
- Evaluating real-time machine data in safety relevant applications
- Developing a generic framework which combines the strengths of KPI-classification and machine learning
  - Machine learning as augmentation

### Case Study

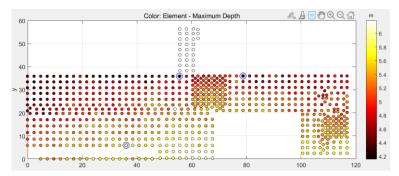
- Vibro replacement ground improvement process
  - Monitored with sensors with n<sub>s</sub>= 16 channels
  - Non-uniform sub-surface conditions from site to site
  - Varying creation time for a single column  $t_c = 6 \dots 30$  min
  - Varying number of MVTS per site m = 400 ... 1000 MVTS
  - Manually performed process

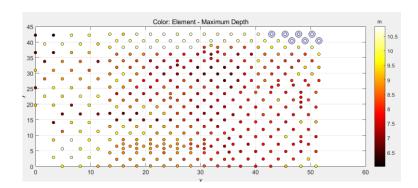
### For each foundation column a MVTS is created

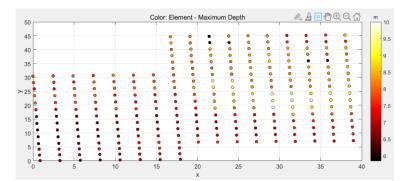


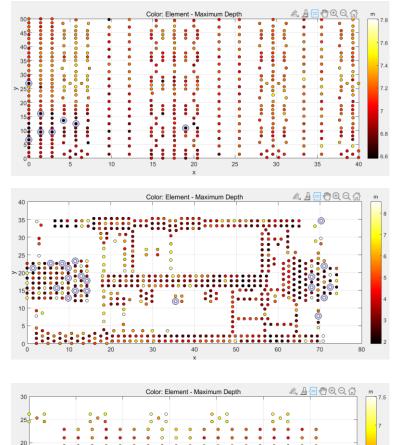


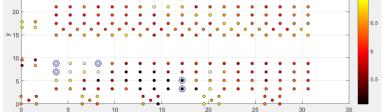
### Geo-referenced KPI for multiple sites









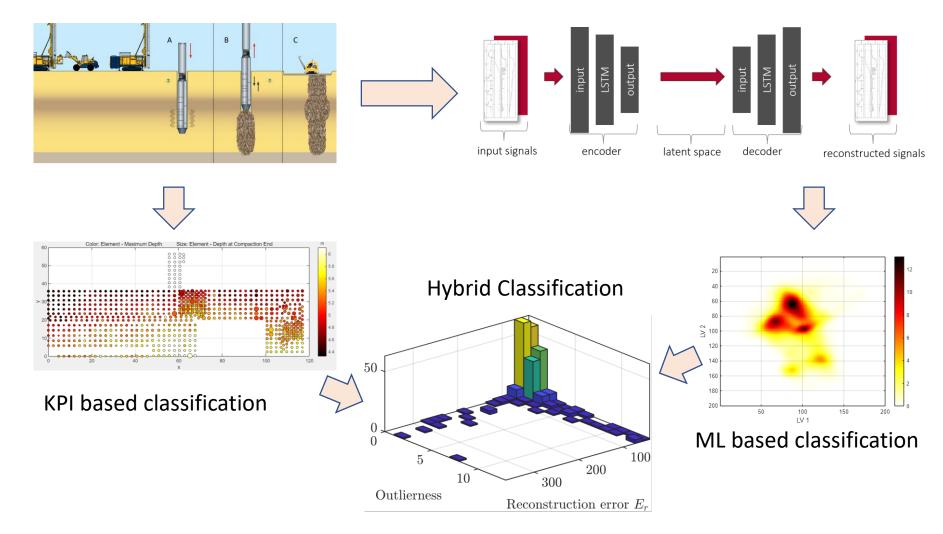




### Overview of the Hybrid Classifier

#### **Physical Process**

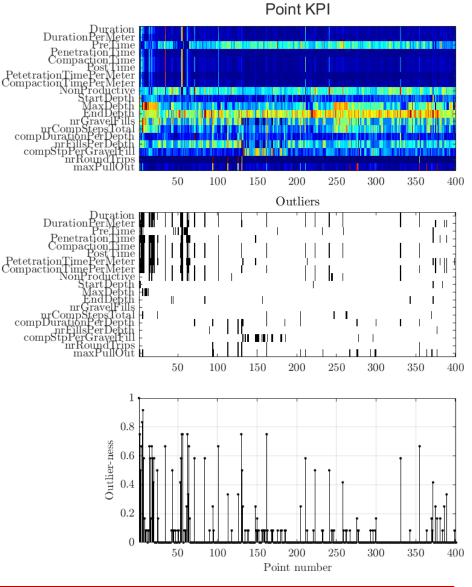
LSTM-VAE

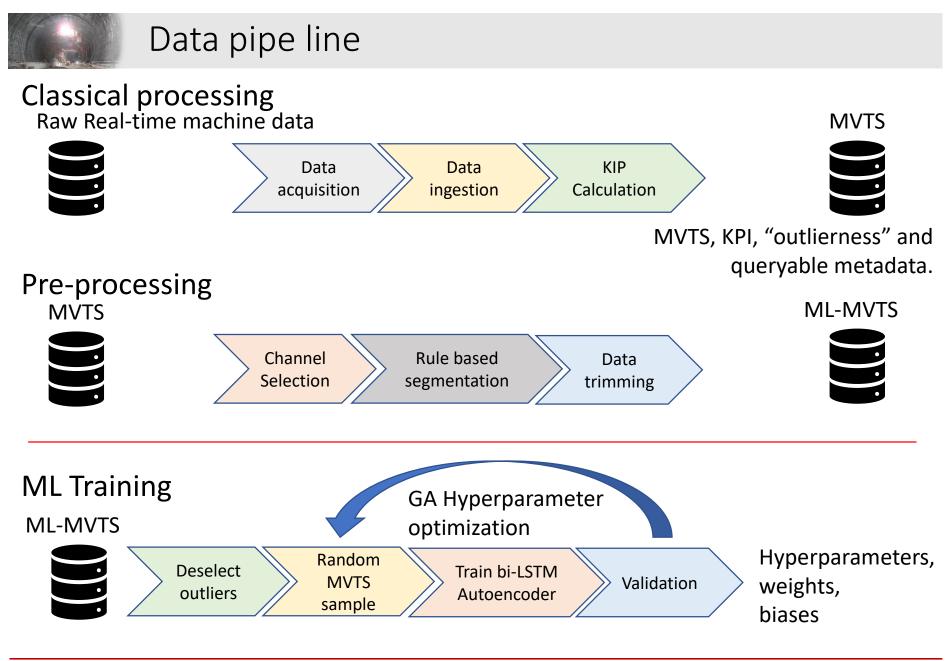




### **KPI-based** classifier

- 49 KPI
- Outlier detection is performed for each sensor channel and each KPI based on IQR
- Outliers values which are outside the lower bound  $b_l$  and the upper bound  $b_u$
- $b_u = q_{75} + 1.5 IQR$
- $b_l = q_{75} 1.5 IQR$
- "Outlierness":
- Artificial word
- Quantification of the degree that a MVTS is an outlier





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## Step 1: Channel Selection for ML

- Different goals may require different selection of channels, e.g., column quality and production efficiency.
- Metadata-based channel selection.

#### Complete data record

#### MMM Depth M www Force 100 Amps 10:04 10:07 10:0510:0610:1010:0810:0910:1110:12Time Mar 11, 2020

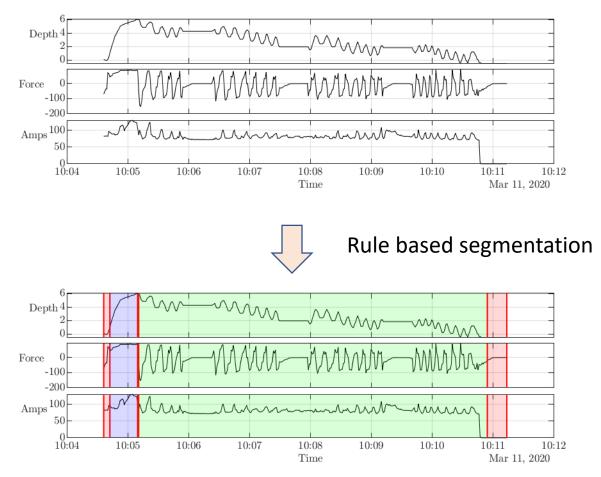
Note: More data channels, does not imply a better model.

# Originally we tested using all the data but the results were not as good as with selected channels.

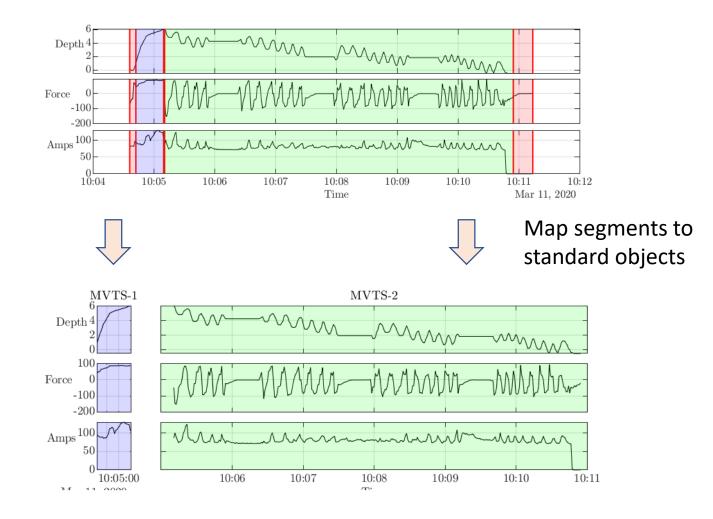
Channels relevant for quality

### Step 2: Rule based segmentation

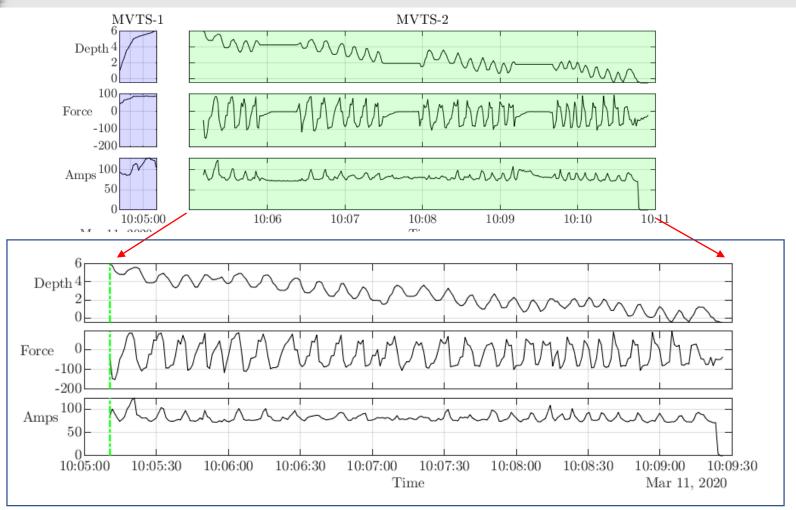
 Expert rules used to segment the data according to subprocesses.



### Step 3: Common data structures used for MVTS



### Step 4: Remove no activity (no change of state)

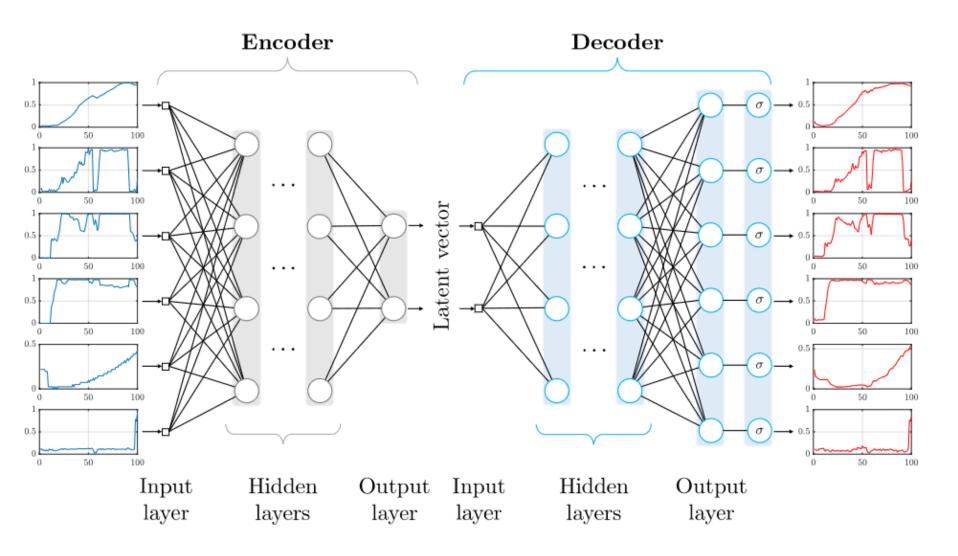


## Result: An MVTS binary object for each column and a corresponding "outlierness" value via the KPI.

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### Basic Autoencoder





# Hybrid Machine Learning

Hybrid classifier consists of two parts:

#### 1) KPI classifier

- Automatic identification of systematic changes in the MVTS
- 2) Unsupervised machine learning classifier
  - Detecting non-linear relationships between the sensor channels
  - Detecting anomalies which were not addressed by the KPI directly
    - Errors that were not considered in the KPI design

- Serial-Parallel hybrid model
  - Combination of the classifications (logical OR)

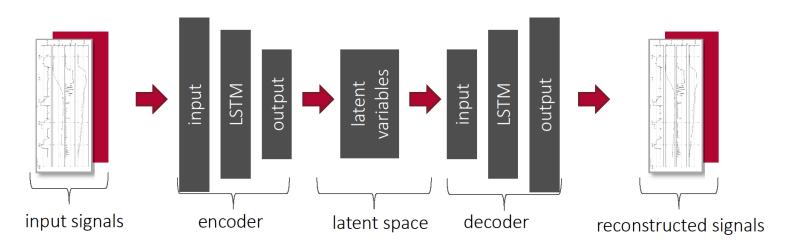
ML

KPI



### ML-based classifier

- LSTM-based variational autoencoder (LSTM-VAE)
  - Performs dimensionality reduction by encoding the input signals into lower dimensional latent variables
  - Variational autoencoder generative model
    - Latent variables: Gaussian distributions with mean and standard deviation



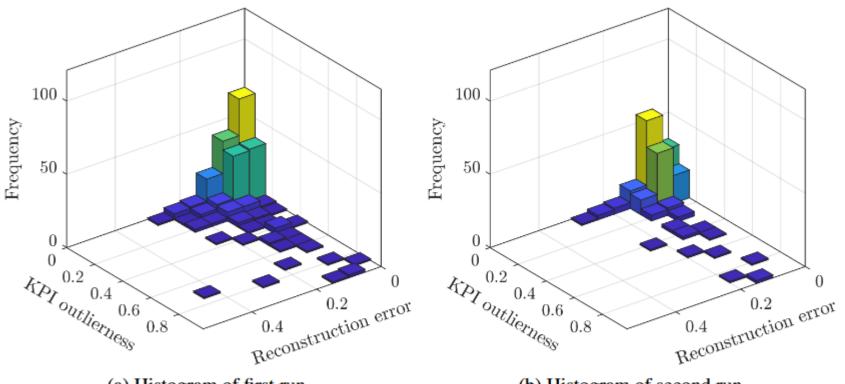
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# Cost Function of the LSTM-VAE Classifier

- $D_{KL}$ : Kullback-Leibler divergence
  - Quantification for the similarity of two distributions
  - Assumes independence of variables/ sensor channels
  - Does not take into account the sequence of the data
  - $E_r$  : reconstruction error:
    - Difference between initial MVTS (input signal) Y with m signals and the reconstructed MVTS  $\widehat{Y}$  (reconstructed signal)
    - $E_r = \sum_{k=1}^m ||Y_k \lambda \hat{Y}_k||_F^2$  with  $\lambda = 1$
- $E_t$ : cost function VAE-LSTM training
  - $E_t = E_r D_{KL}\{N(0,1) | | N(\mu, \sigma)\}$



# Bivariate: "outlierness" vs ML-Reconstion error



(a) Histogram of first run

(b) Histogram of second run

Fig. 7.15: Bivariate histograms of the reconstruction error and the outlierness obtained with KPIs. The training was performed with unlabeled data via 4-fold cross-validation, and the average test error was computed for each sample. For the second run the anomalous samples found in the first run were eliminated from the data set.



# Comparison of sub-process performance

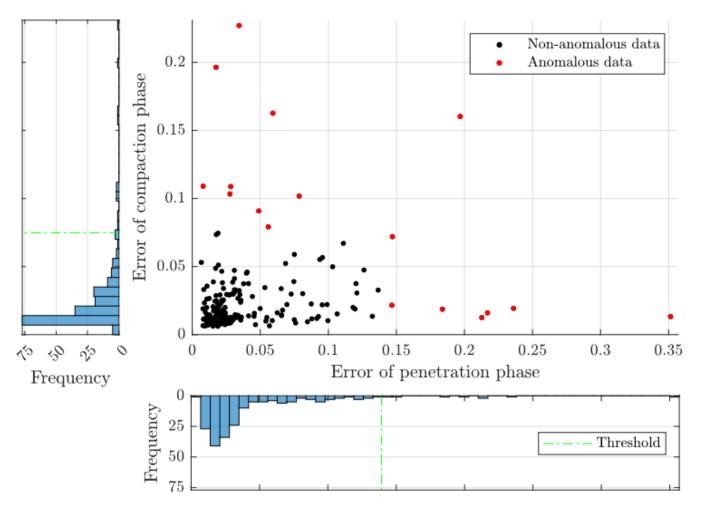
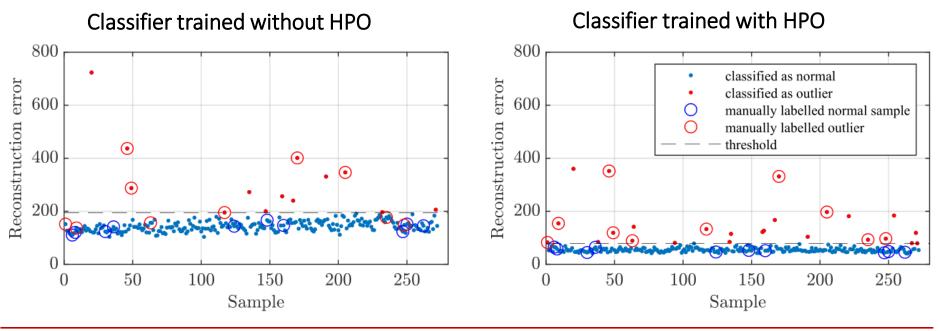


Fig. 7.16: Phasewise error plot of test data samples, with corresponding histograms of the error distributions and threshold values for separating normal data from outliers.

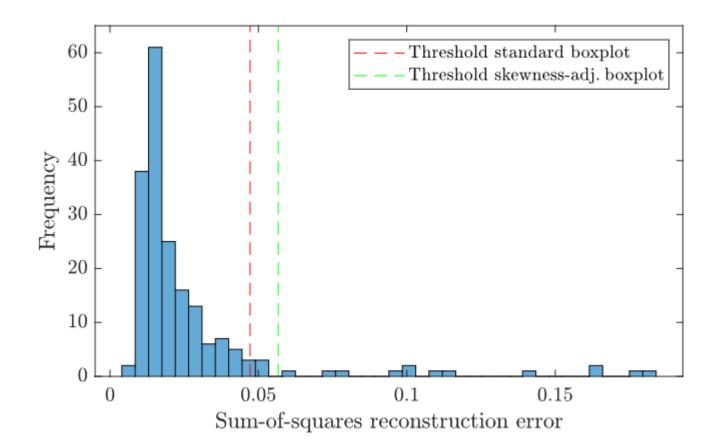
# Importance of Hyperparameter Optimization (HPO)

- Improved reconstruction error for classifier trained with optimized hyperparameters
  - Higher distance between the labelled groups of outliers and normal samples
  - Lower variance and IQR within the groups tighter bounds for the detection of outliers
  - No false classifications of the manually labelled examples after the hyperparameter optimization



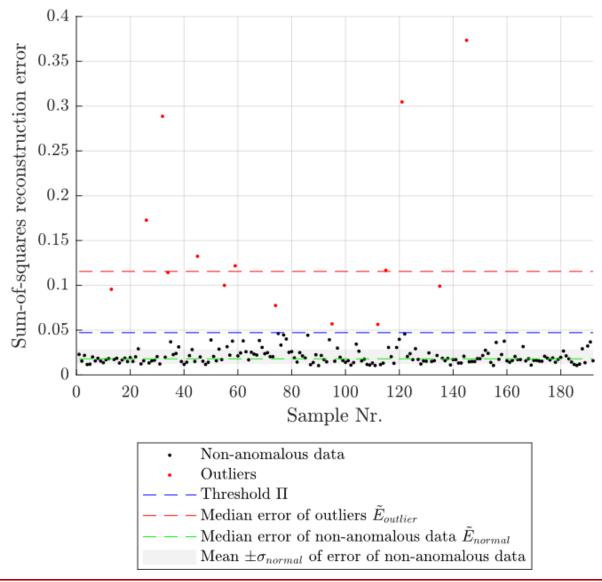


### Skewness adjustment





#### ML Classification





# Hyperparameter Optimization (HPO)

#### Settings of the Genetic Algorithm:

Latent dimension: 3

Population size: 20

Maximum number of generations: 7

Mutation probability: 0.05

Random probability: 0.05

 Table 1: Results of HPO with 1-layer networks

Data:

Site: Fehring

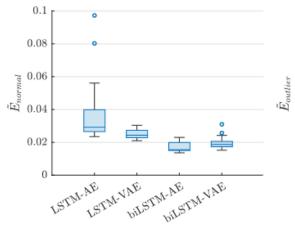
Number of input channels: 6

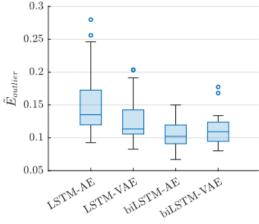
Number of training samples: 80

Network Structure			Optimized Hyperparameters					
Net Type	Layer Encoder	Layer Decoder	Nr. Epochs	Neurons Encoder	Neurons Decoder	Learning Rate	Batch Size	
			[1, 100]	[1, 100]	[1, 100]	[3·10 <sup>-3</sup> , 1·10 <sup>-1</sup> ]	[2, 53]	
AE	LSTM	LSTM	93	59	19	3.691·10 <sup>-2</sup>	12	
VAE	LSTM	LSTM	77	55	30	5.133·10 <sup>-2</sup>	4	
AE	biLSTM	biLSTM	96	70	32	1.877·10 <sup>-2</sup>	3	
VAE	biLSTM	biLSTM	96	57	47	2.571·10 <sup>-2</sup>	6	

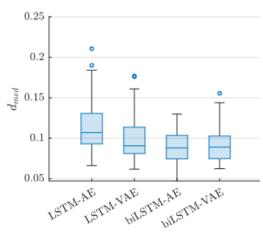


# Comparing different architectures



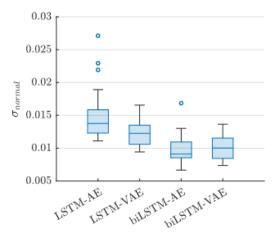


(a) Median error of samples labeled as non-anomalous



(c) Distance of median errors of non-anomalous samples (a) and anomalous samples (b)

(b) Median error of samples labeled as anomalous



(d) Standard deviation of errors of samples labeled as non-anomalous

Fig. 7.7: Statistical measures of sum-of-squares sample errors obtained with different autoencoder architectures containing one hidden layer in encoder and decoder for  $n_{runs} = 25$  test runs.



### Comparing LSTM and bi-LSTM

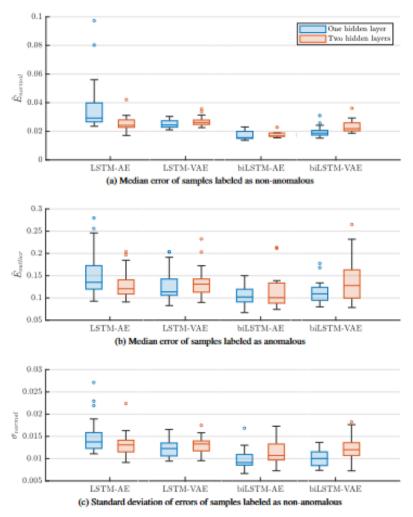


Fig. 7.9: Statistical measures of sum-of-squares sample errors obtained with different autoencoder architectures for n = 25 test runs. The boxplots in blue are associated with autoencoders, whose encoder and decoder contain one hidden layer. The boxplots in orange correspond to autoencoders, whose encoders and decoders contain two hidden layers.

# Run dependent performance vs architecture

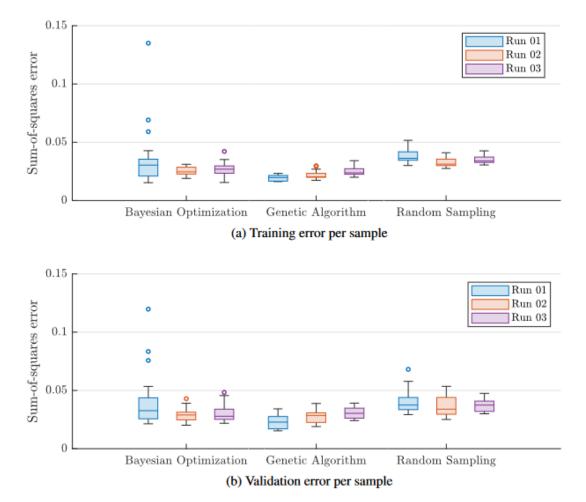


Fig. 7.10: Sum-of-squares errors per sample of training samples (a) and validation samples (b) after the last epoch for biLSTM-AEs. The hyperparameters were optimized  $n_{HPO} = 3$  times with each of the tested HPO methods, and with each hyperparameter configuration  $n_{runs} = 25$  test runs were performed.



#### Comparison of Weight Initializers

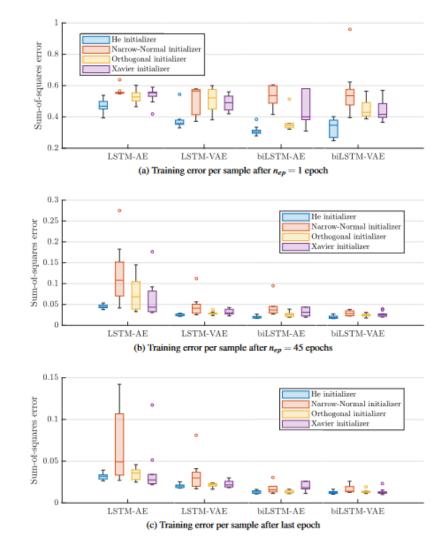


Fig. 7.12: Boxplots of sum-of-squares training error per sample of different autoencoders after a particular number of epochs using four different weight initializing methods. For each method and autoencoder  $n_{runs} = 10$  runs were performed.

# Comparison of Weight Initializers

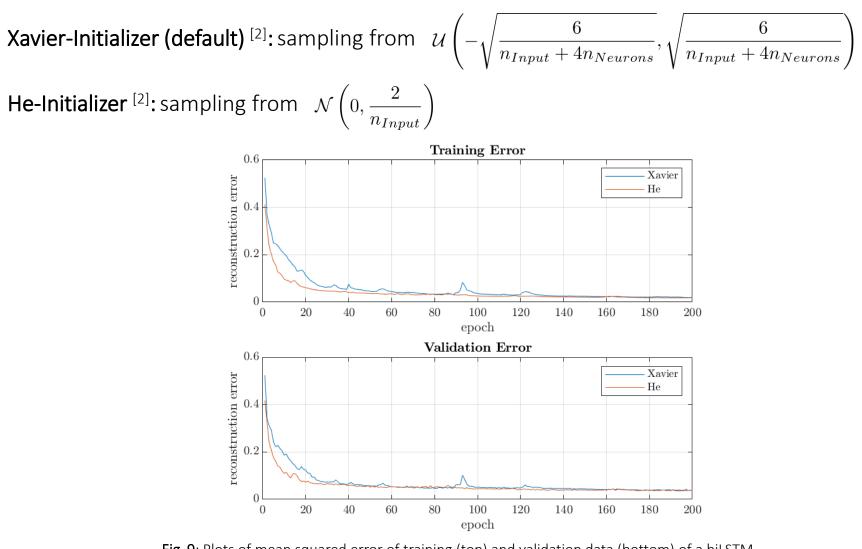


Fig. 9: Plots of mean squared error of training (top) and validation data (bottom) of a biLSTMbiLSTM VAE with different weight initializers

# Statistical behaviour of the different architectures

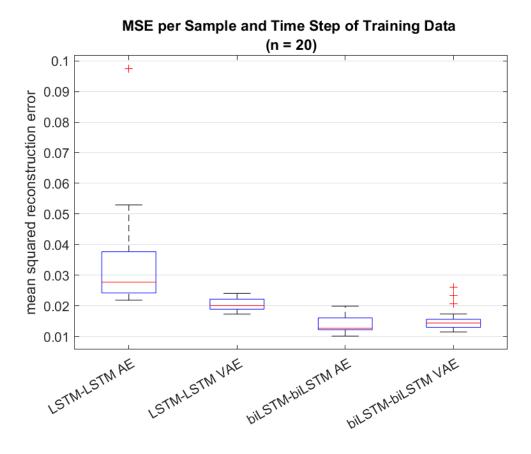


Fig. 10: Boxplot of MSE per sample and time step with training data as input



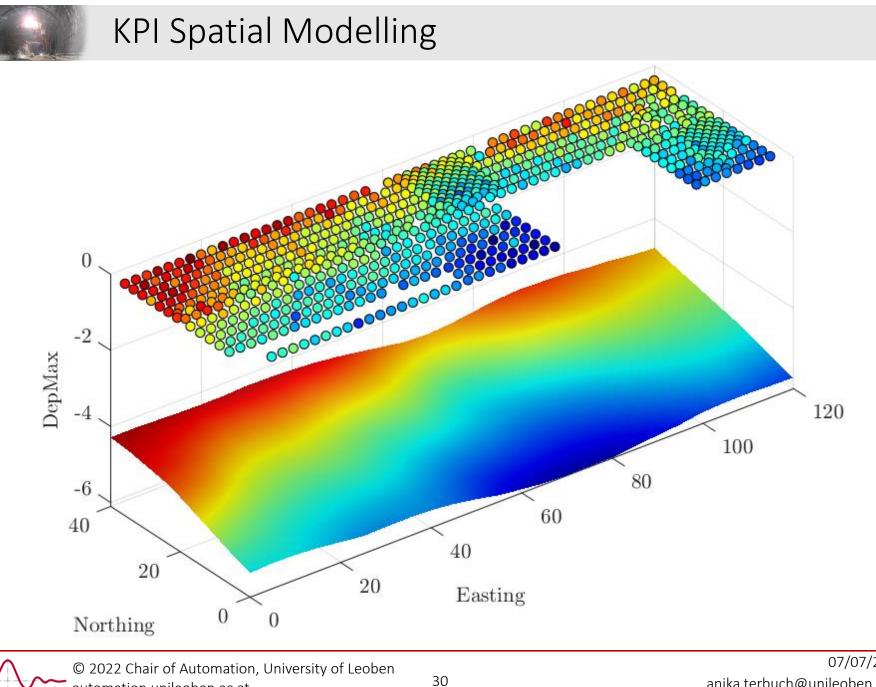
#### Table 2: Results of HPO with 1-layer networks – first and obsolete run

Network Structure			Optimized Hyperparameters					
Net Type	Layer Encoder	Layer Decoder	Nr. Epochs	Neurons Encoder	Neurons Decoder	Learning Rate	Batch Size	
Range			[1, 100]	[1, 100]	[1, 100]	[5e-5, 1e-2]	[2, 2/3 x n <sub>Samples</sub> ]	
AE	LSTM	LSTM	92	75	96	8.22e-3	13	
VAE	LSTM	LSTM	88	97	71	9.28e-3	5	
AE	biLSTM	biLSTM	83	70	32	9.51e-3	3	
VAE	biLSTM	biLSTM	82	62	65	7.83e-3	12	



#### Further work

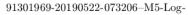
- Alternative cost function / measures in the latent space
- Serial-parallel-hybrid model
  - Pre-selecting the MVTS for training the ML-classifier using KPI-analysis
- Incorporating other normalizations for the sensor signals
- Including other variables (e.g. the latent dimension) in the hyperparameter optimization
- Subsurface modelling to separate systematic from random variations to improve outlier detection via KPI.

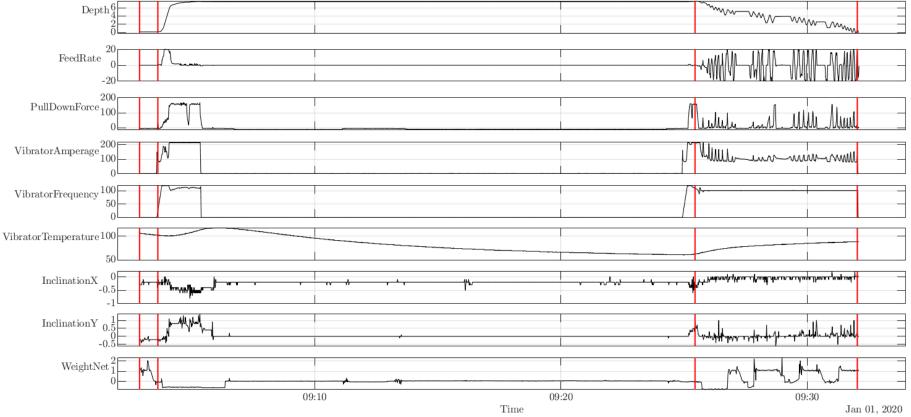


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# Classified as outlier by both

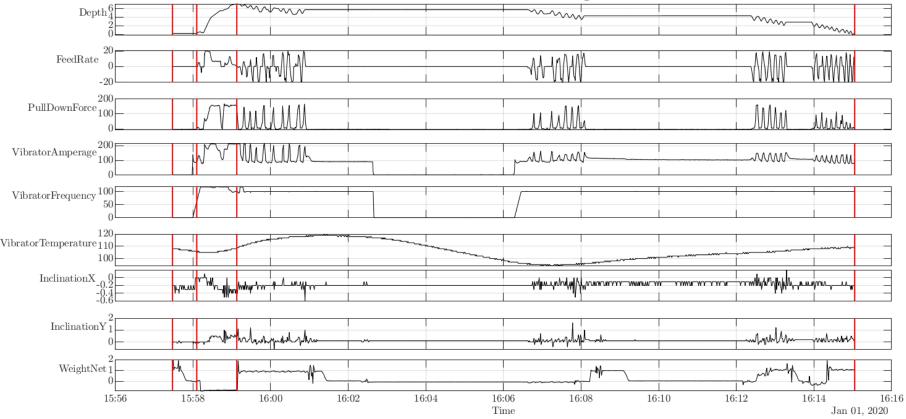








# Classified as outlier by ML



91301969-20190529-141503-M5-Log-



# Classified as outlier by KPI

