

# Set Functions for Time Series

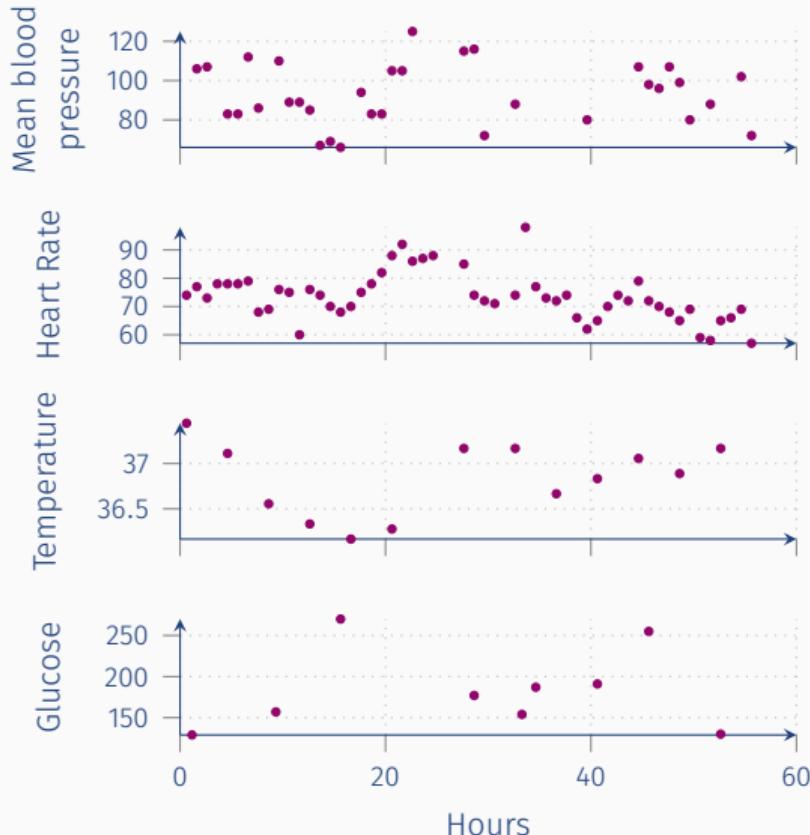
ICML 2020

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Max Horn, Michael Moor, Christian Bock, Bastian Rieck and Karsten Borgwardt

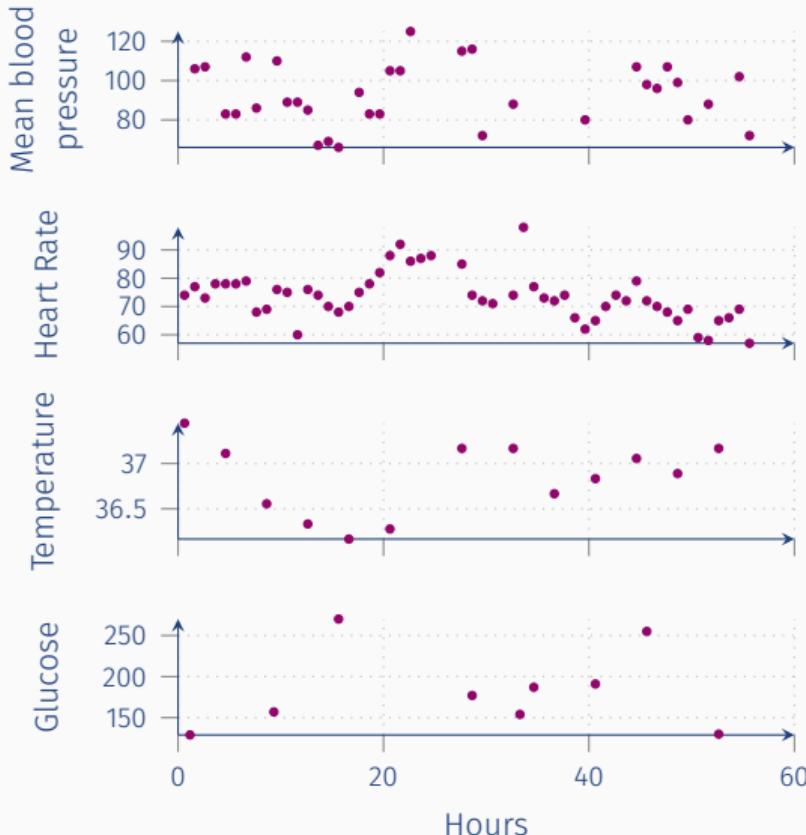
Machine Learning and Computational Biology Group, ETH Zurich

# Motivation - Medical time series



Challenges

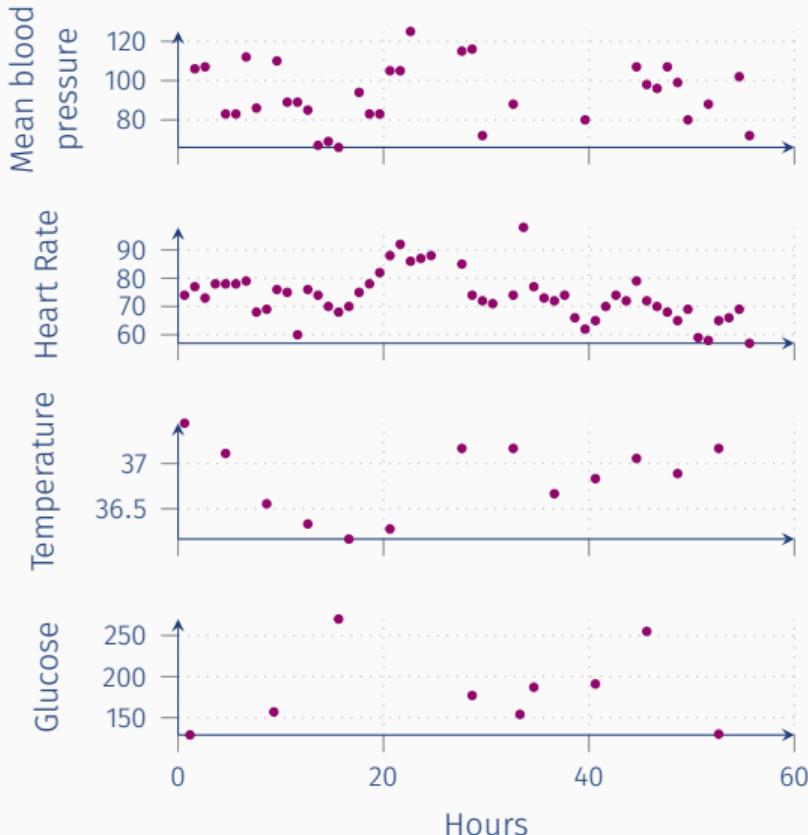
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## Challenges

- Irregular sampling of data

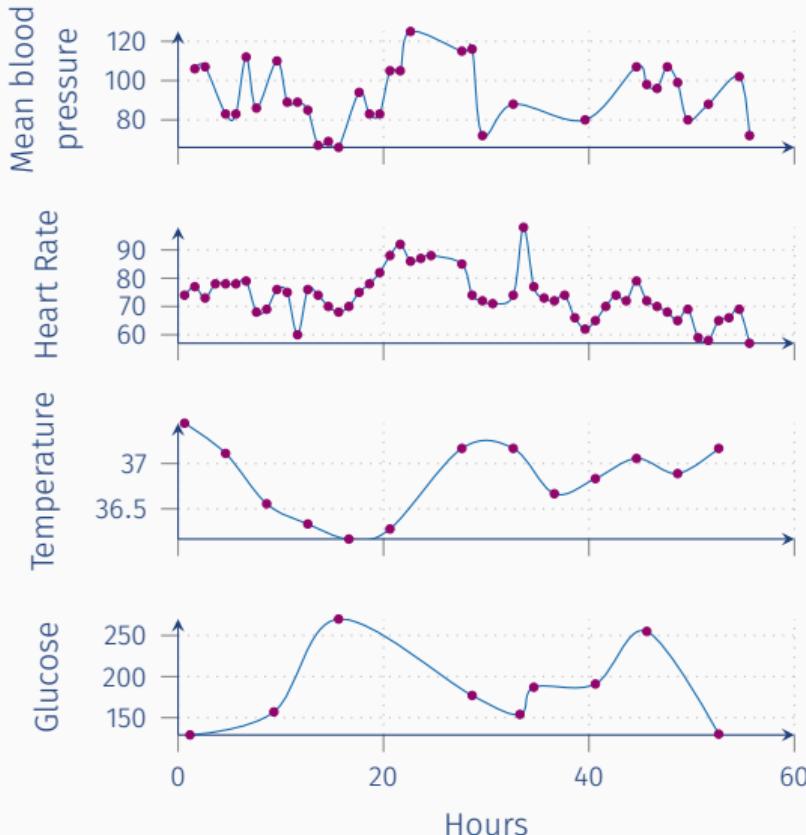
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## Challenges

- Irregular sampling of data
- High demands on interpretability

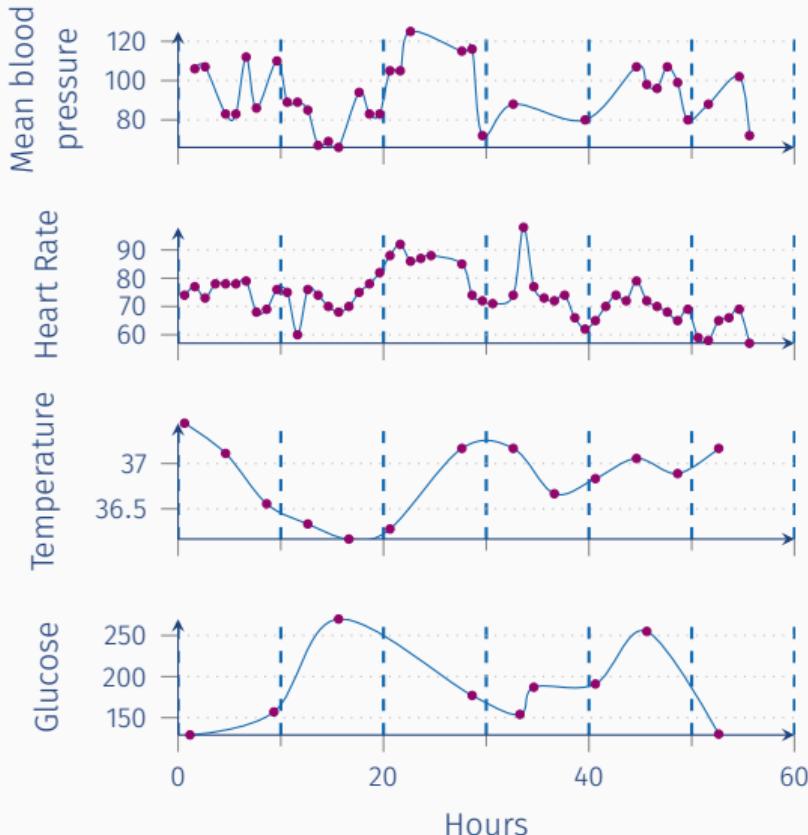
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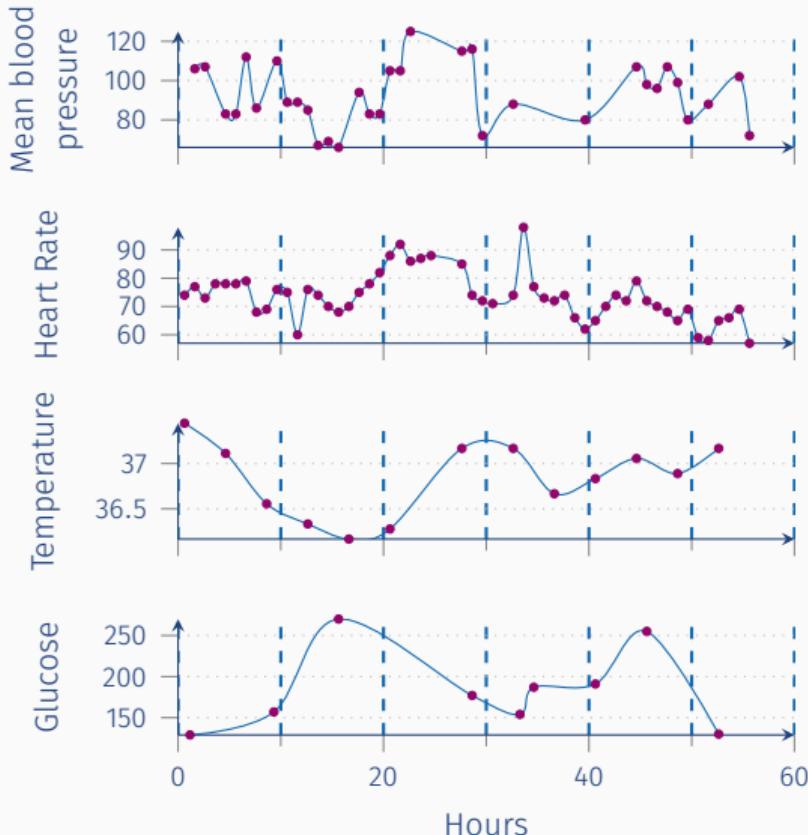
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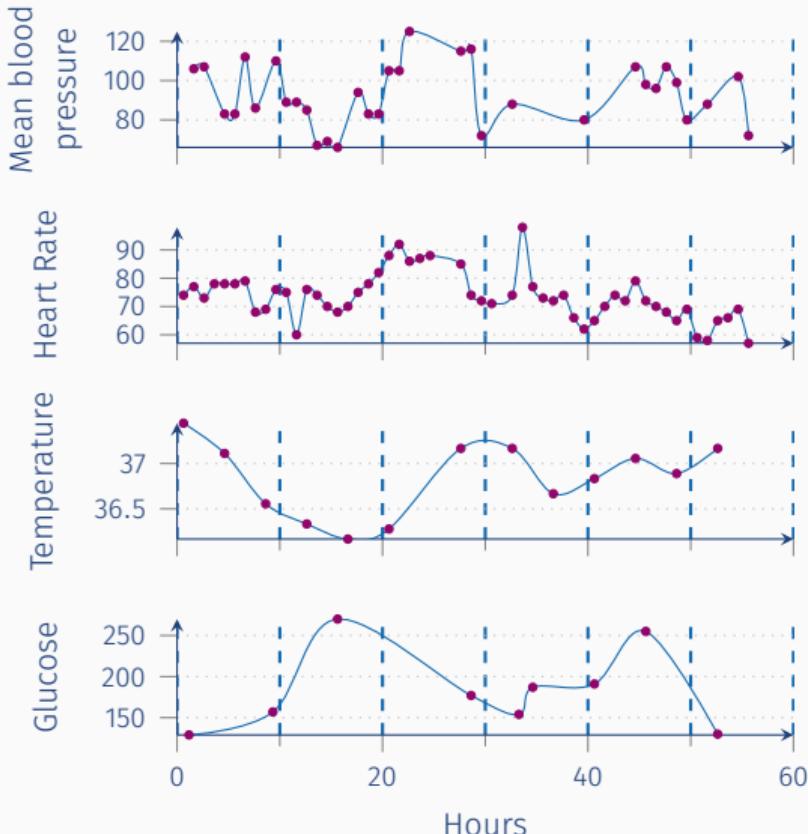
## Challenges

- Irregular sampling of data
- High demands on interpretability

## Problem statement

Learning classification models on irregularly-sampled time series without prior imputation.

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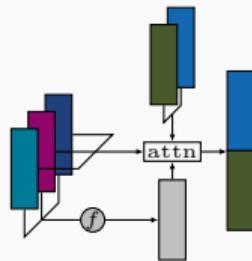
Learning classification models on irregularly-sampled time series without prior imputation.

## Set Functions for Time Series

→ Time series classification as set classification

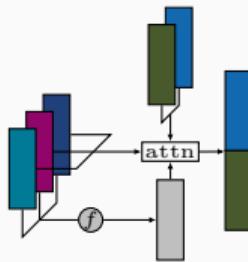
# Contributions

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New approach for  
Irregularly-sampled Time  
Series

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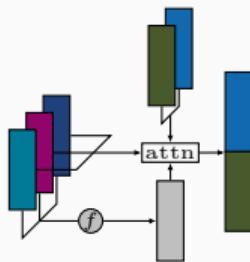


New approach for  
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Competitive Performance  
with Lower Runtime

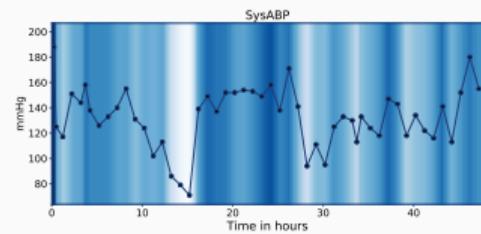
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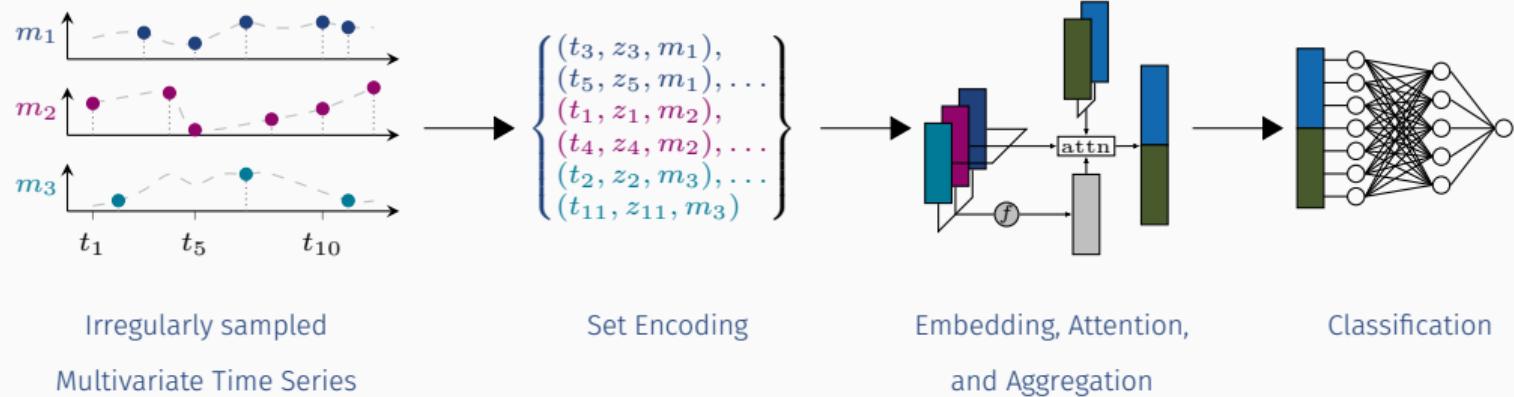


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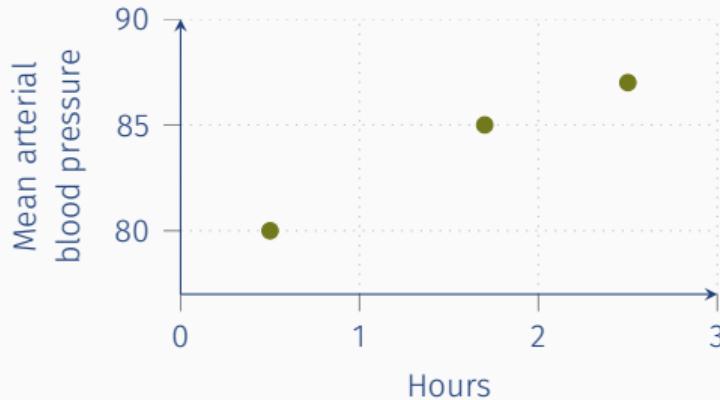
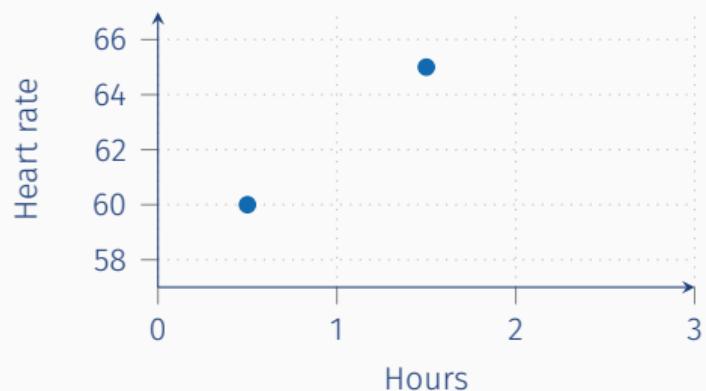


Per Observation  
Contributions

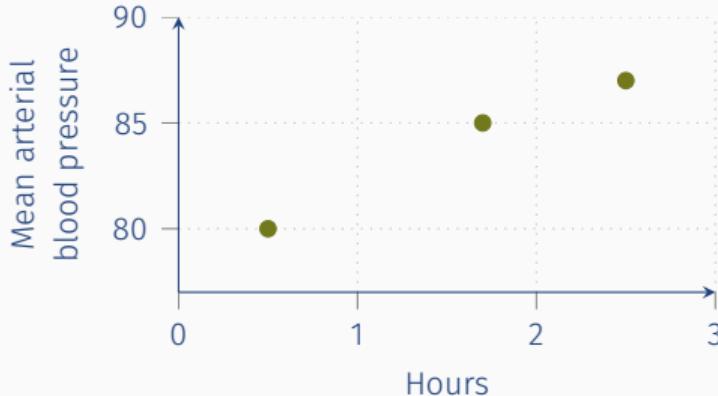
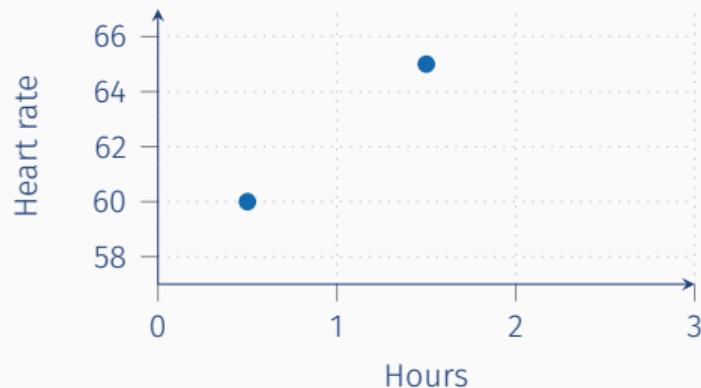
# Architecture Overview



## Key idea - Time Series as Sets of Observations

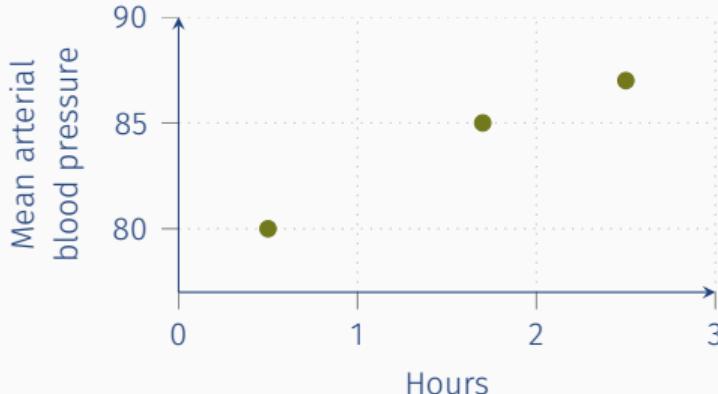


## Key idea - Time Series as Sets of Observations



Each observation  $s_j$  is represented as a tuple  $(t_j, z_j, m_j)$

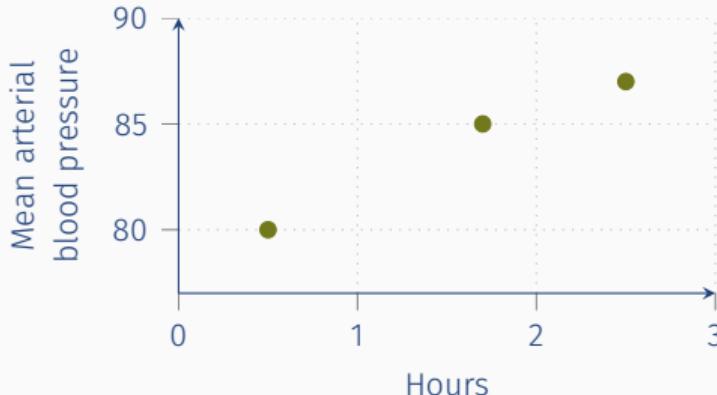
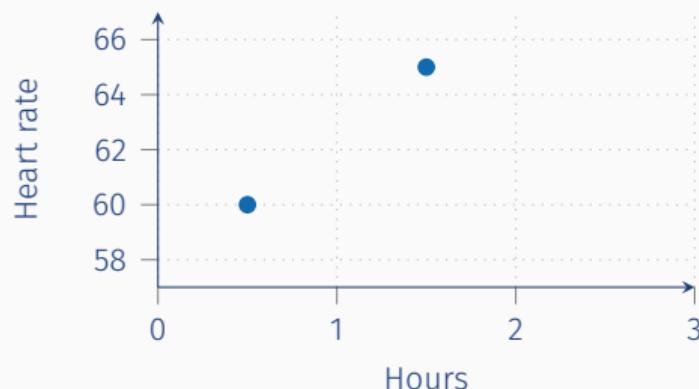
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$$\mathcal{S} = \{(0.5, 60, 1), (1.5, 65, 1),$$

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$$\mathcal{S} = \{(0.5, 60, 1), (1.5, 65, 1), (0.5, 80, 2), (1.7, 85, 2), (3, 87, 2)\}$$

# Deep Sets<sup>1</sup>

$$f(\mathcal{S}) = g\left(\frac{1}{|\mathcal{S}|} \sum_{s_j \in \mathcal{S}} h(s_j)\right)$$

where  $h: \Omega \rightarrow \mathbb{R}^d$  and  $g: \mathbb{R}^d \rightarrow \mathbb{R}^C$  are neural networks

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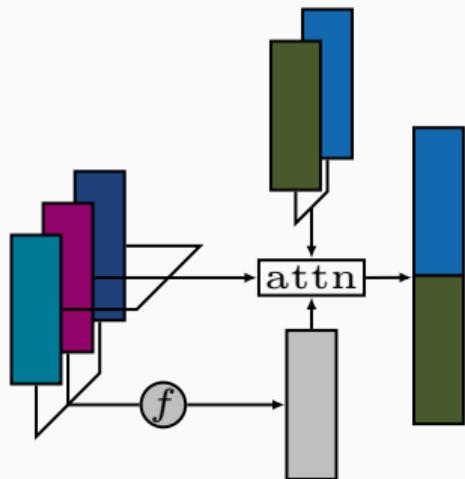
## Problem

Influence of an element shrinks as  $|\mathcal{S}|$  grows!

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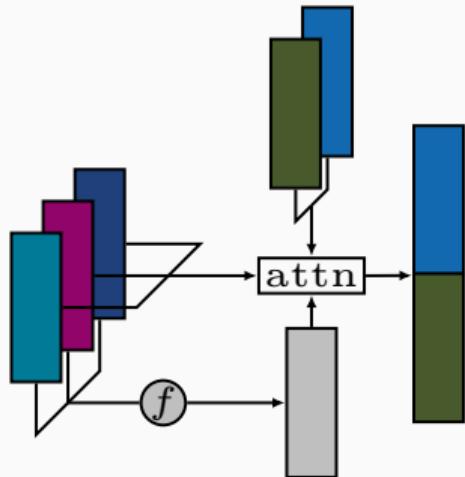
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## Set Attention Mechanism

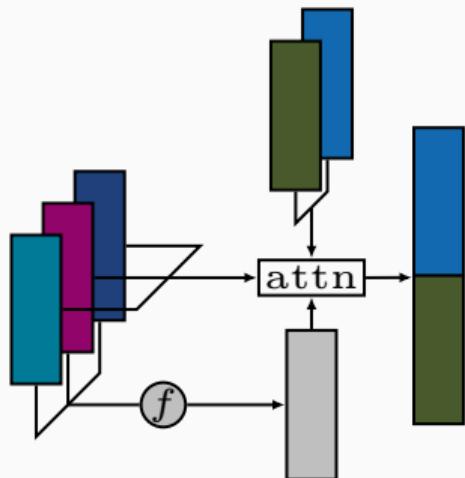


# Set Attention Mechanism

$$\text{Keys: } K_{j,i} = [f(\mathcal{S}), s_j]^T W_i$$



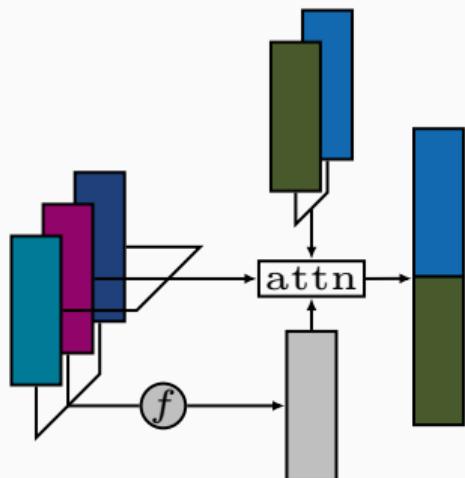
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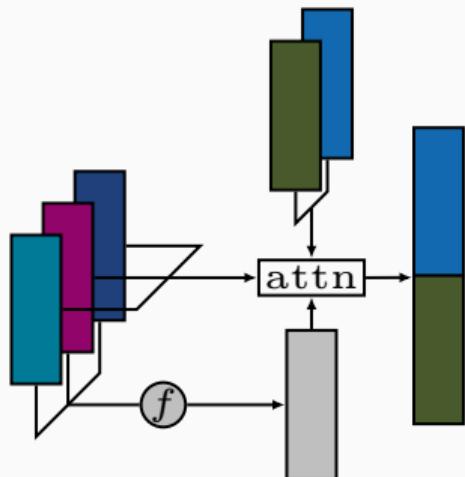


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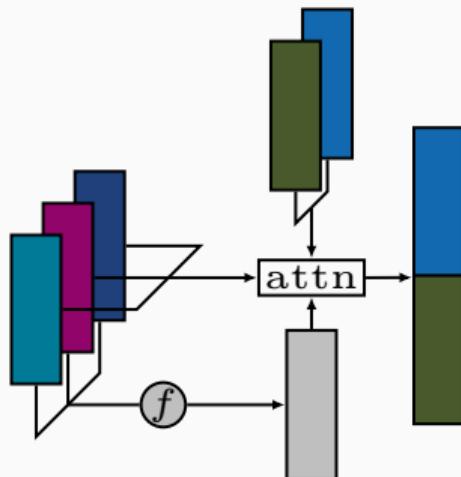
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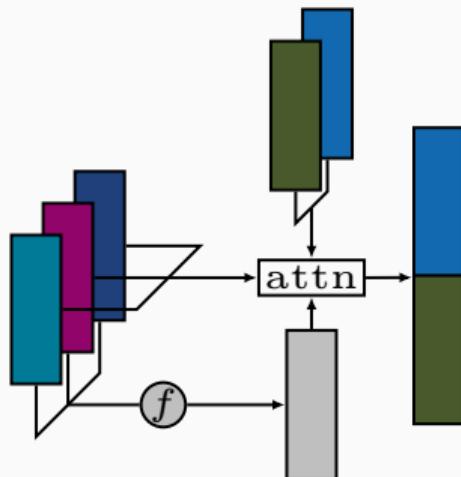
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Values:  $V_i = \sum_j a_{j,i} h_\theta(s_j)$

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$$\mathcal{L}(\theta, \psi) = \mathbb{E}_{(\mathcal{S}, y) \in \mathcal{D}} \left[ \ell \left( y; g_\psi \left( \sum_{s_j \in \mathcal{S}} a(\mathcal{S}, s_j) h_\theta(s_j) \right) \right) \right]$$

# Experimental setup

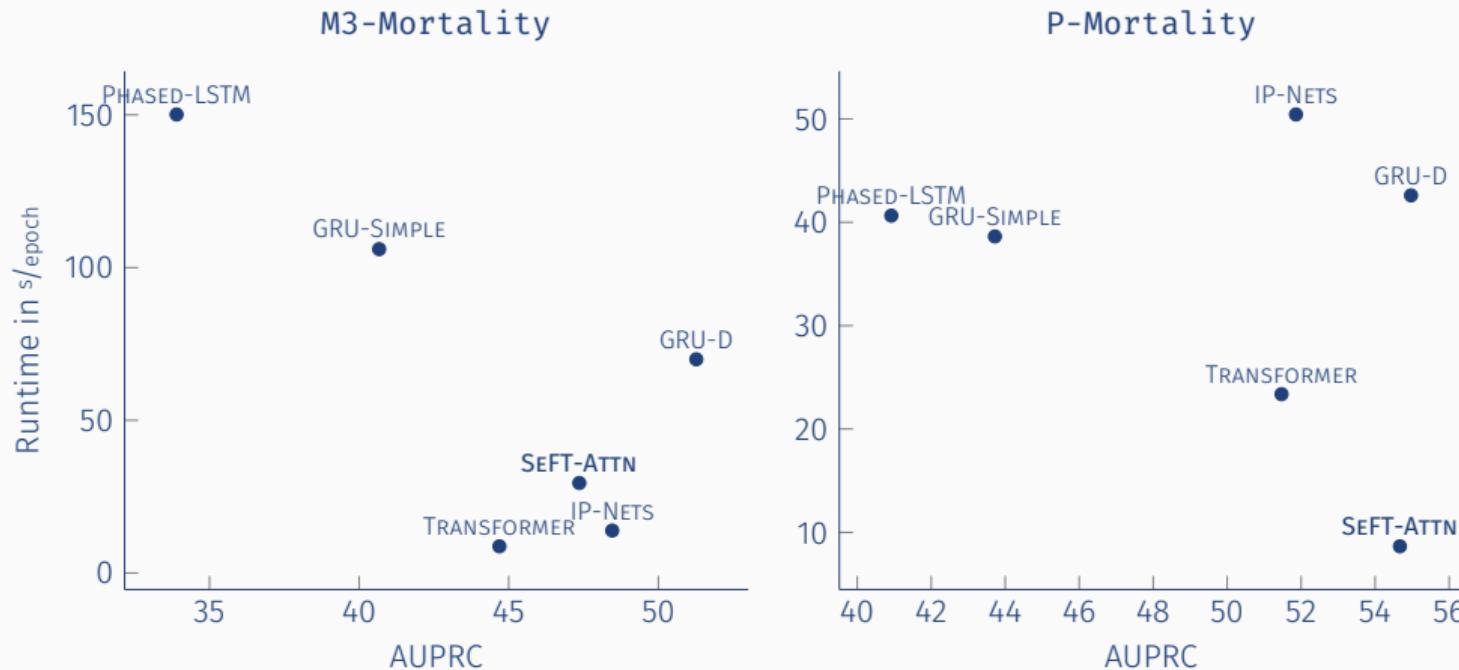
## Datasets

- Two mortality prediction tasks - MIMIC-III (**M3-Mortality**) and Physionet 2012 (**P-Mortality**)
- Sepsis early recognition task - Physionet 2019 Challenge

## Comparison partners

- PHASED-LSTM – *Neil et al., NeurIPS 2017*
- TRANSFORMER – *Vaswani et al., NeurIPS 2017*
- GRU-SIMPLE & GRU-D – *Che et al., Scientific reports 2018*
- IP-NETS – *Shukla & Marlin, ICLR 2019*

# Results - Performance vs. Runtime



## Results - Sepsis Early Prediction

Model	B-Accuracy	AUPRC	$U_{\text{norm}}$	s/epoch
GRU-D	51.15	5.82	0.02121	190.41
GRU-SIMPLE	50.69	6.97	0.01309	92.90
IP-NETS	<b>78.02</b>	<b>37.60</b>	<b>0.51327</b>	232.92
PHASED-LSTM	50.09	6.40	0.00159	110.49
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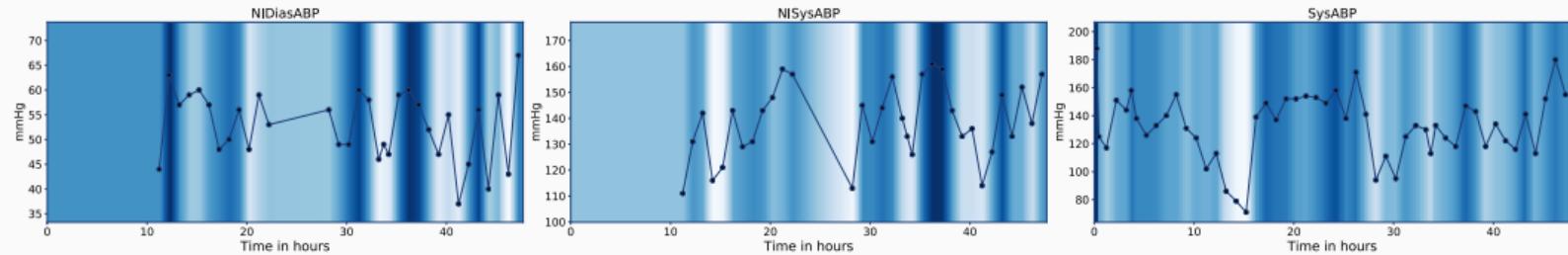
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## Possible Leakage of Future Information

**IP-NETS** Through unmasked interpolation

**TRANSFORMER** Through layer normalization

## Results - Interpretability



Uniquely allows a **per-observation** quantification of importance

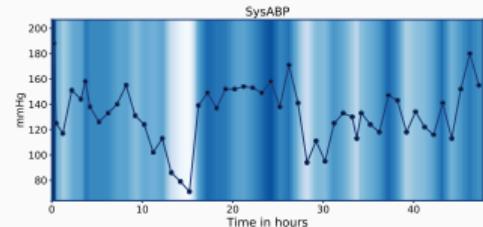
# Summary

$$\left\{ \begin{array}{l} (t_3, z_3, m_1), \\ (t_5, z_5, m_1), \dots \\ (t_1, z_1, m_2), \\ (t_4, z_4, m_2), \dots \\ (t_2, z_2, m_3), \dots \\ (t_{11}, z_{11}, m_3) \end{array} \right\}$$

New approach for  
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Competitive performance  
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Per observation  
contributions

For further information please check out our paper.

