Sustainable advanced manufacturing via machine learning-assisted exploitation of sensing and data infrastructure

Transforming Foundation Industries Network+ Conference

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December 5, 2023

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Project Overview

Aims and Objectives

Aim of the Collaboration

- **Aim**: To develop integral data acquisition and analytics frameworks that leverage expert process knowledge with ML techniques. This will yield informed data infrastructure design guidelines that **will accelerate the uptake of ML in the manufacturing process**.

Technical Challenges

1. Development of Quantitative Framework

- Industrial processes governed by complex multi-stage physical systems that rely on sequential decision making
- Current ML activity not focused on this type of processes: **data scarcity**
- Define new metrics that capture the performance specifications in a framework that is compatible with ML techniques

2. Optimal Process Monitoring and Feature Identification

- **Information density** estimation to characterise evidence provided by parameter to yield performance
- Identification of **optimal parameters and sampling times** to maximise utility of monitoring data
- Characterisation of parameter ranges that result in high yield
- Novel **data acquisition infrastructure guidelines** to upgrade industrial plants for efficient operation

3. Prediction of Manufacturing process performance

- ML capability poses demands sensing and data acquisition infrastructure
- Effectiveness of the data capability analysis and ML implementation methodology

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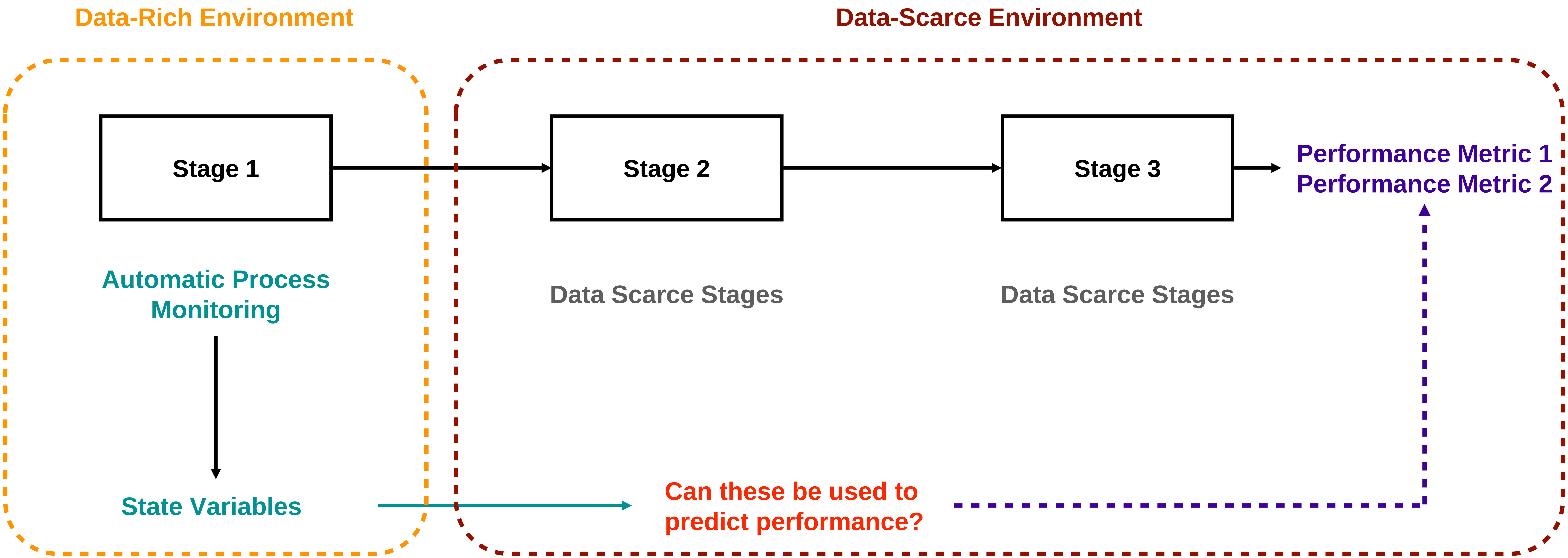
Optimal Process Monitoring and Feature Identification

Project Outcomes



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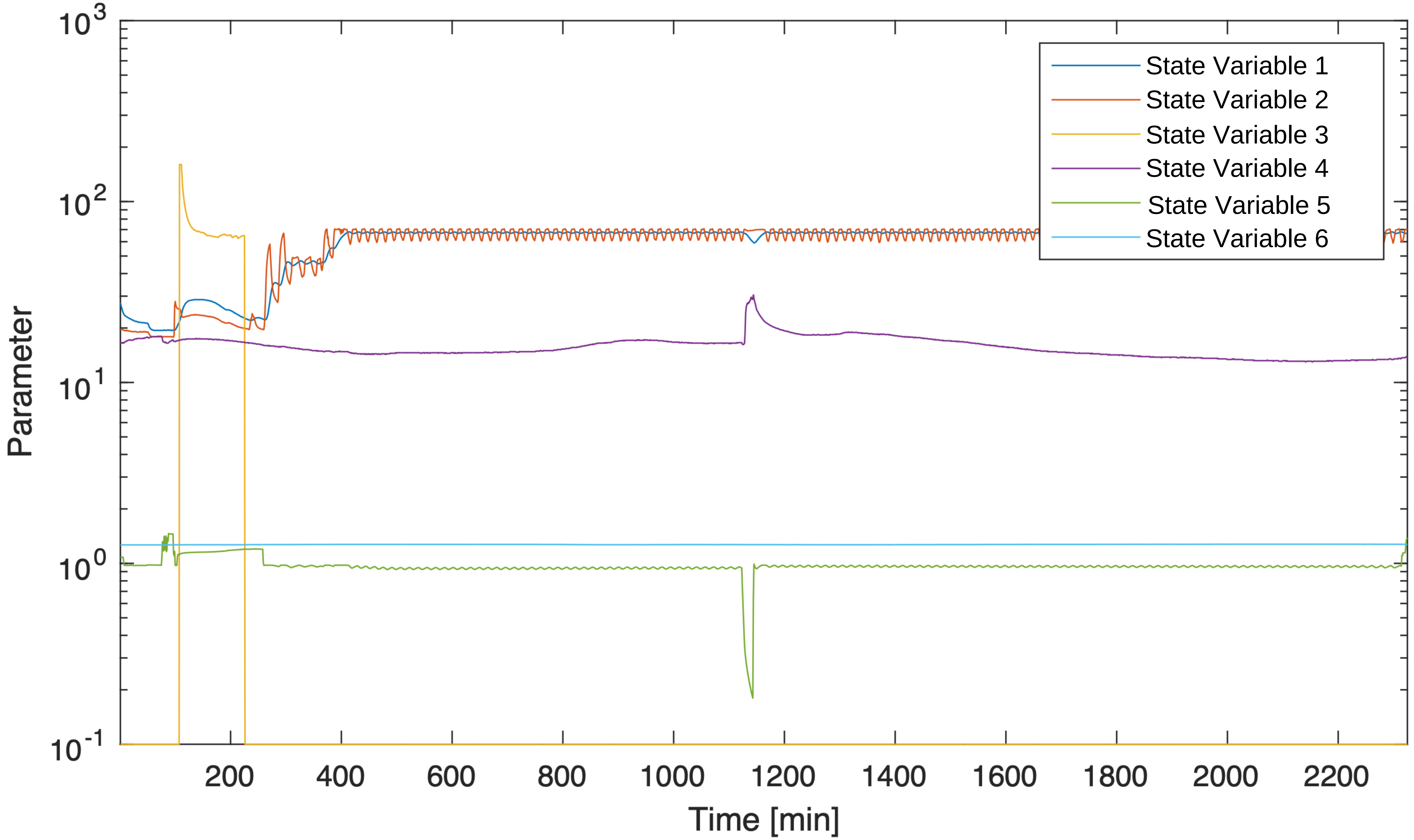
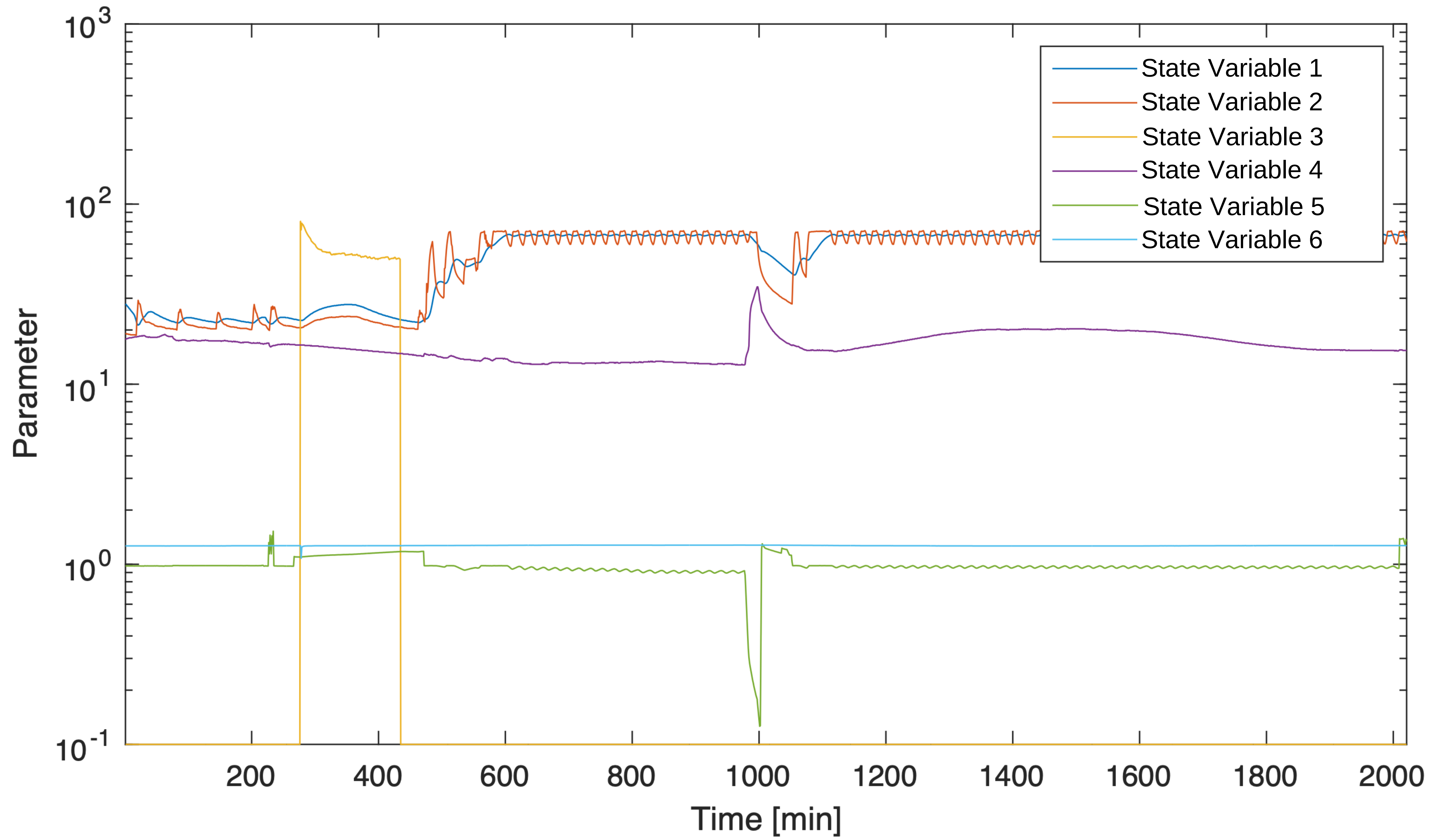
Optimal Process Monitoring and Feature Identification

Example of batch 1



Optimal Process Monitoring and Feature Identification

Example of batch 2



Optimal Process Monitoring and Feature Identification
Parameter Feature Identification Approaches

What are the parameter features that *best* describe the process performance?

- **Approach 1: Relying on visual inspection of to describe features**
  - Finding features that can be geometrically described in terms of the time-series characteristics.
  - Performance is poor, identification relies on **human pattern recognition**: humans require in general more data samples to overcome bias.
  - Solution is **not scalable**: visualisation in high-dimensional settings is challenging.
  - Solution is **not systematic:** extending it to a different process or data source is not straightforward.

- **Approach 2: Mathematical definition of features describing the process parameter time-series**
  - The time-series contain ~2000 samples per batch: cannot be used in as features in raw format.
  - Classical statistical features provided poor performance.
  - Ad-hoc human pattern recognition did not provide desired performance.

- **Approach 3: Information-Theoretic definition of features**
  - We use information measures to **quantify the amount of evidence** provided by the time-series at each time instant.
  - The proposed features can be **ranked** according to the value they provide for yield/ash estimation.
  - **Operational insight** from time-series
    - Dynamical *value of data* assessment.
    - Parameter data storage assessment.

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Optimal Process Monitoring and Feature Identification

Mutual Information

Stochastic Model

- Parameter we wish to estimate: $X \sim \mathbb{P}_X$
- Time-series available to perform estimation: $\left\{(Y_i^{(1)}, Y_i^{(2)}, Y_i^{(3)}, Y_i^{(4)}, Y_i^{(5)}, Y_i^{(6)}\right\}_{i=1}^{n} \sim \mathbb{P}_Y$
- Joint probability distribution: $\left\{X, (Y_i^{(1)}, Y_i^{(2)}, Y_i^{(3)}, Y_i^{(4)}, Y_i^{(5)}, Y_i^{(6)}\right\}_{i=1}^{n} \sim \mathbb{P}_{XY}$

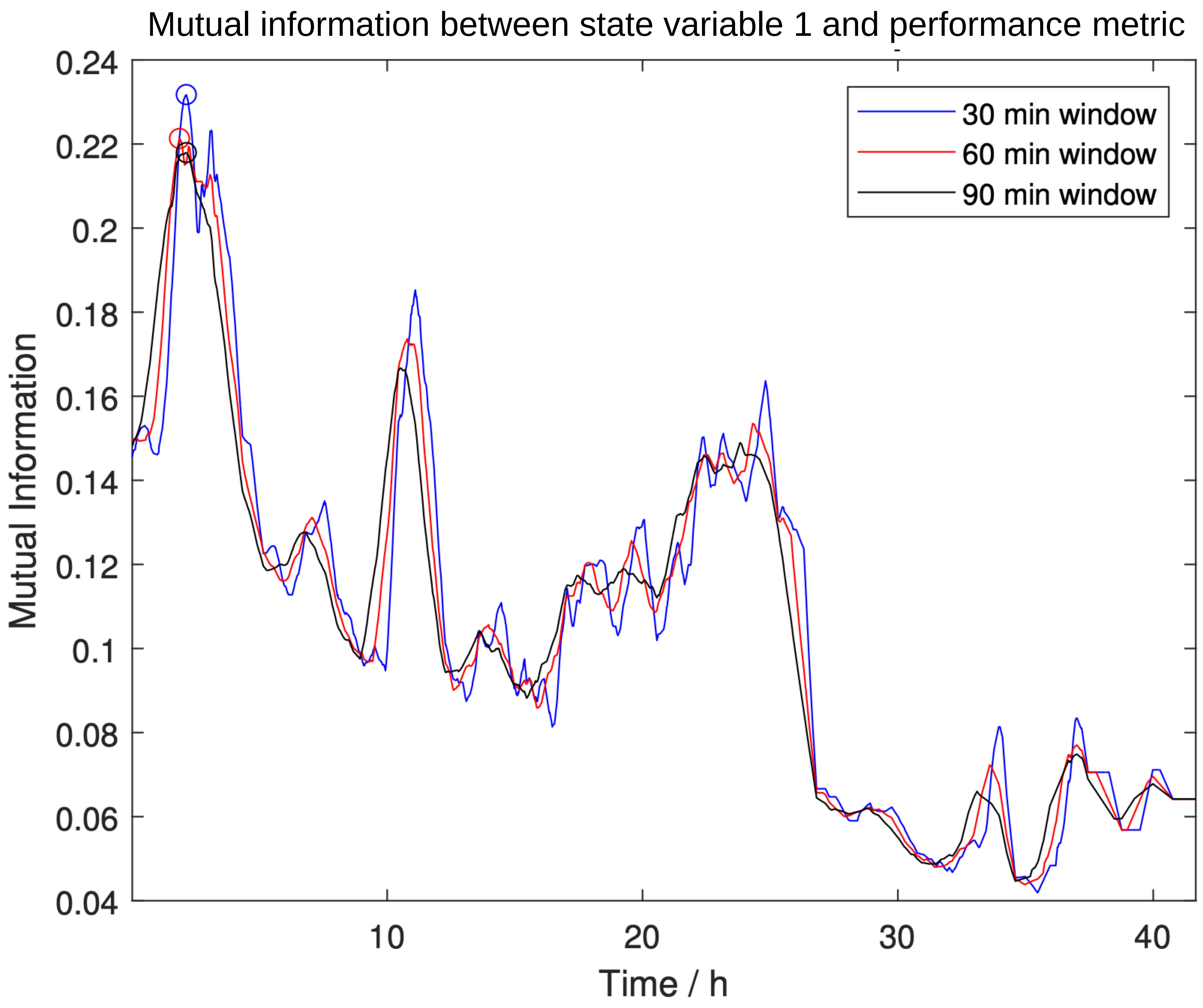
Information Density

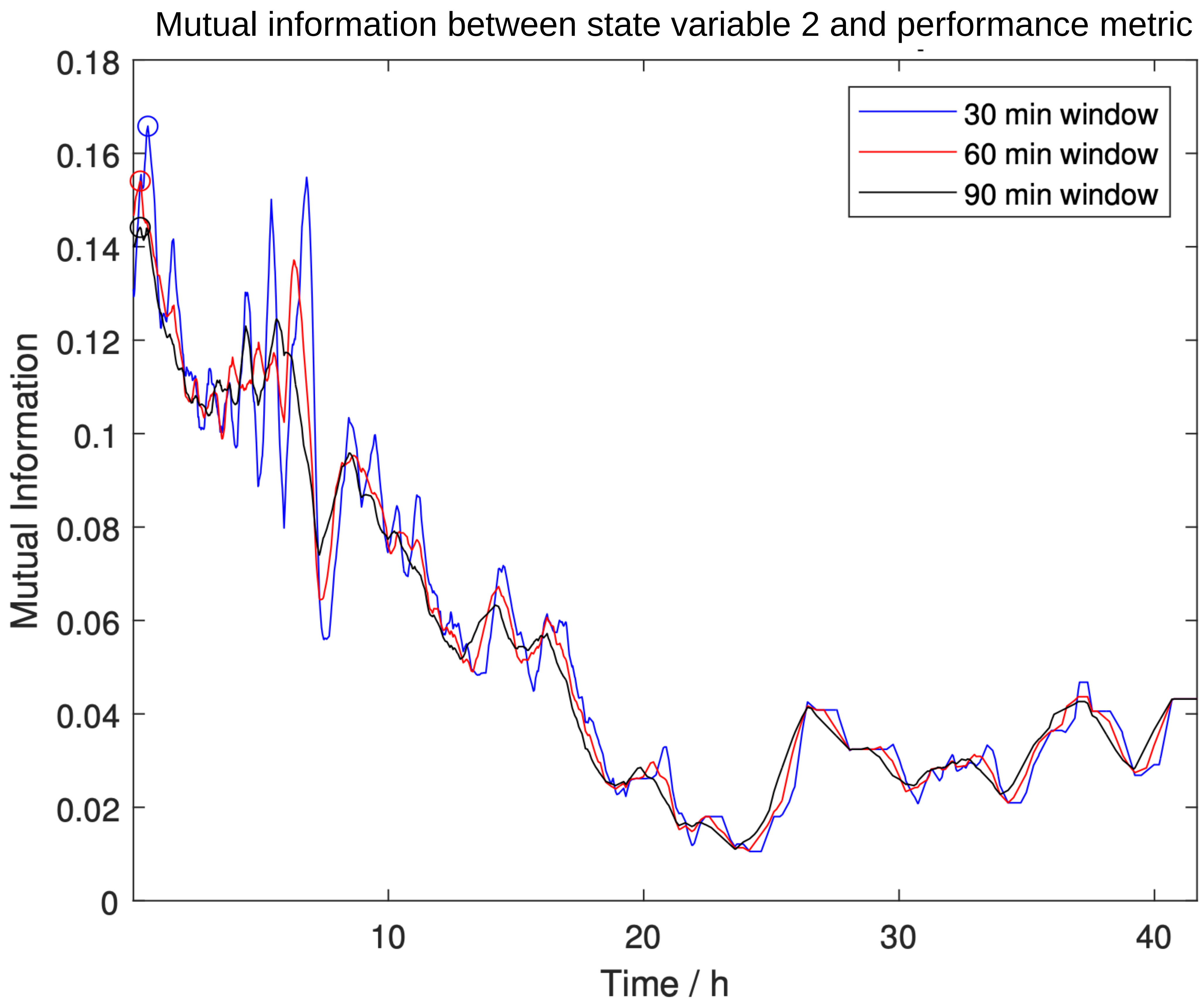
- We compute the **mutual information** at each time instant to evaluate the evidence provided by the parameter k data at each time instant:

$$\boxed{\mathrm{Information}(Y_i^{(k)} \to X) = \int \log\left(\frac{d\mathbb{P}_{Y_i^{(k)}X}}{d\mathbb{P}_{Y_i^{(k)}}\mathbb{P}_X}\left(X, Y_i^{(k)}\right)\right) d\mathbb{P}_{Y_i^{(k)}X}}$$

Numerical Evaluation of Mutual Information

Analysis of Performance Metric 1





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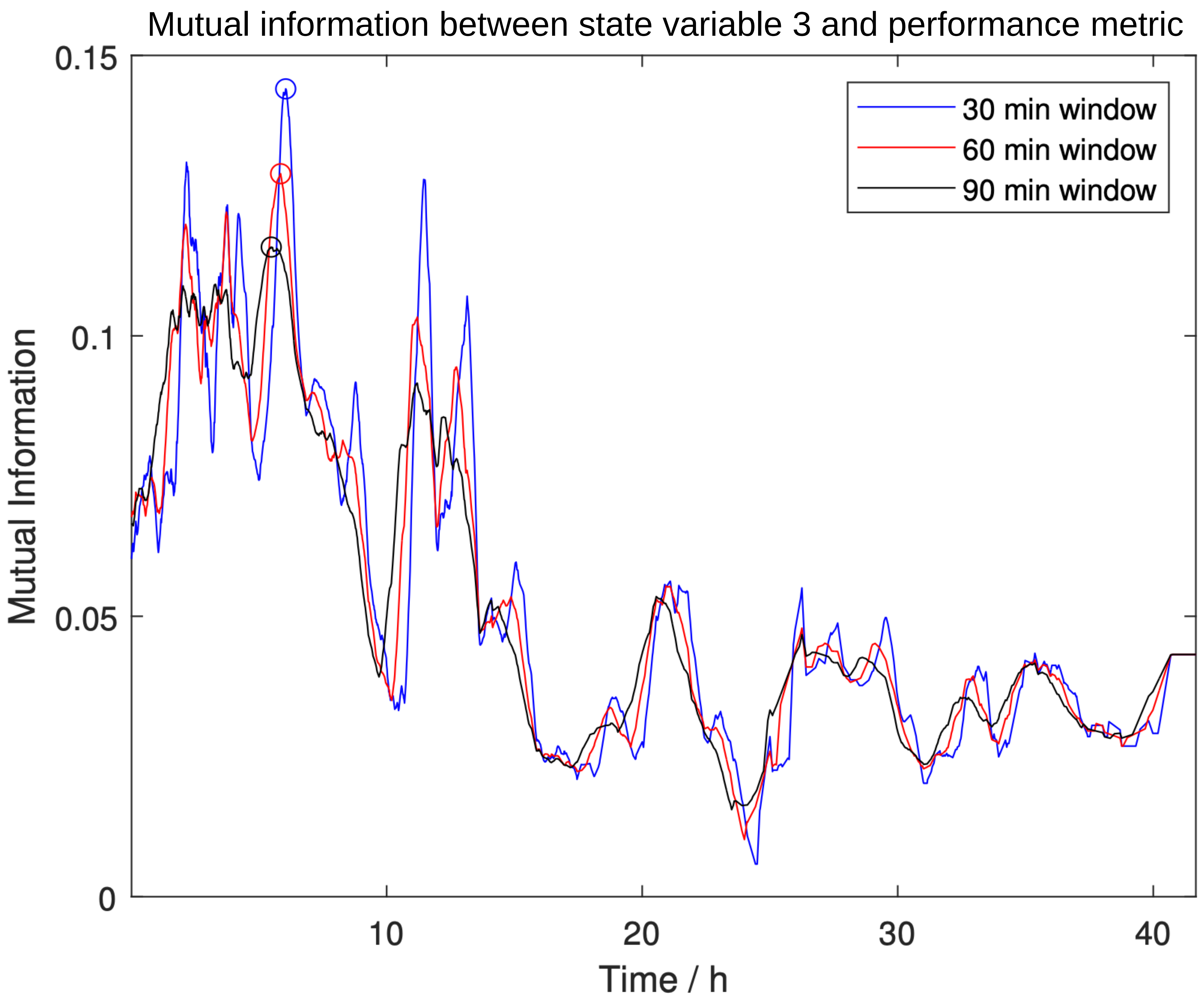
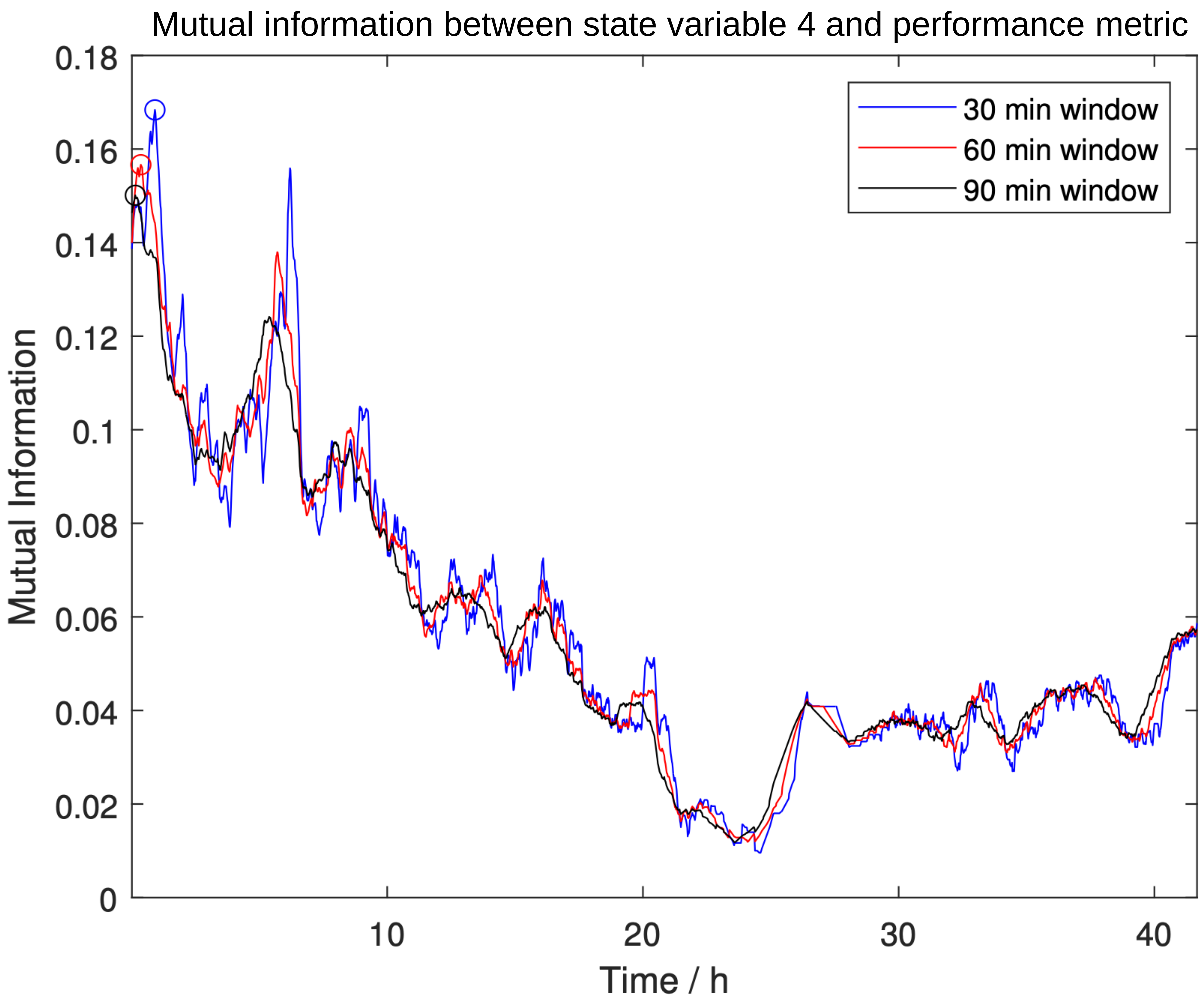
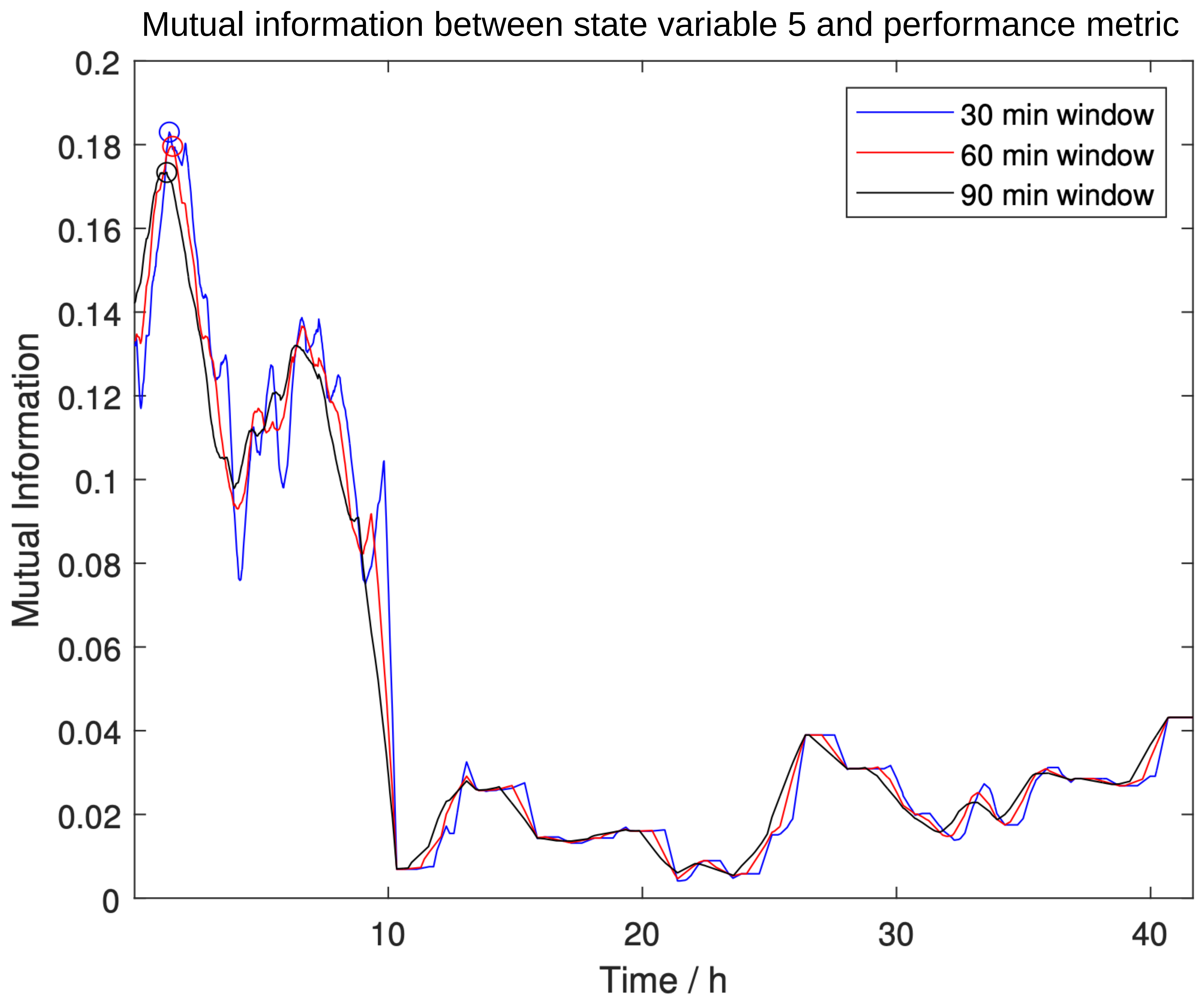
Numerical Evaluation of Mutual Information

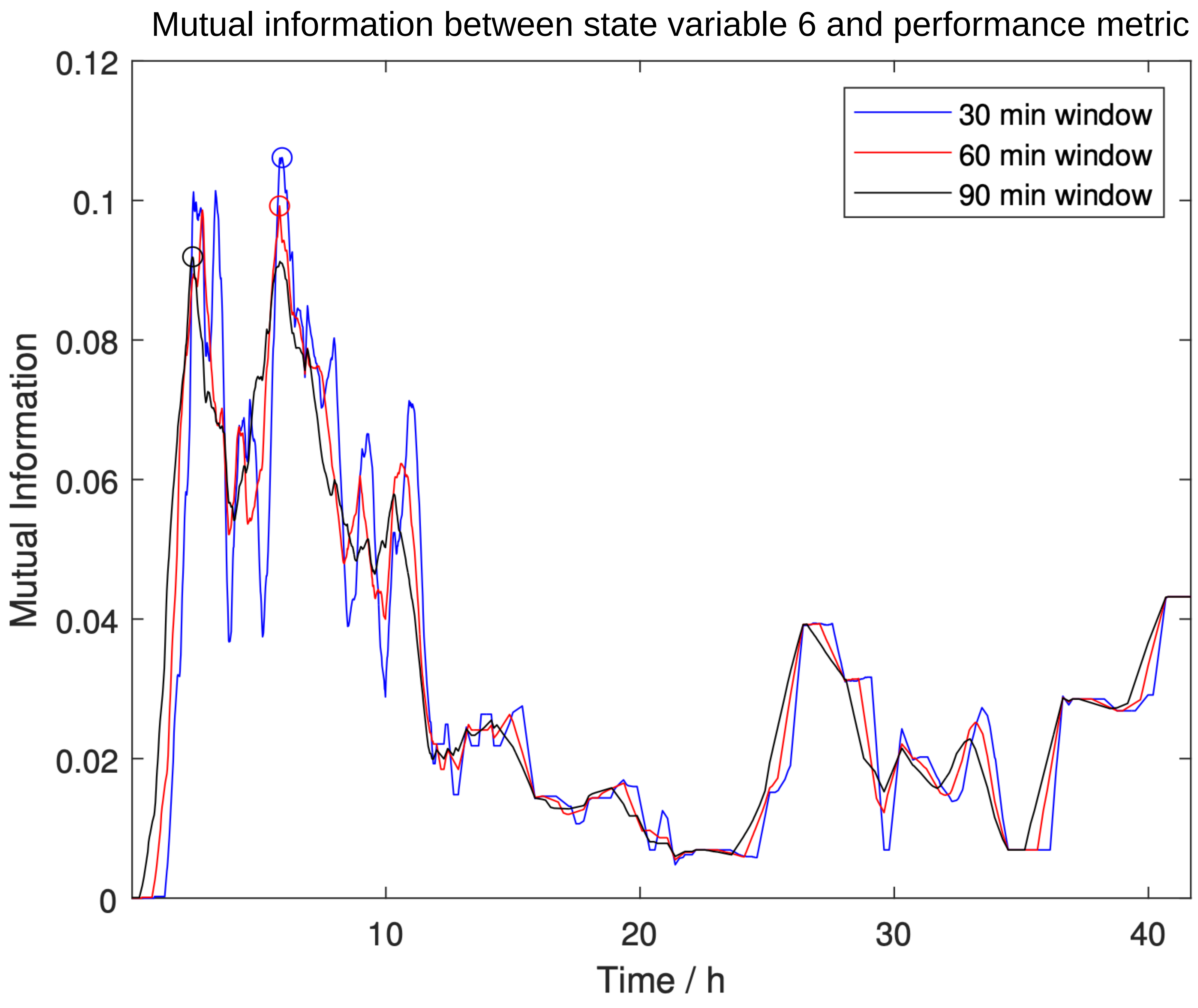
Analysis of Performance Metric 1





Numerical Evaluation of Mutual Information
Analysis of Performance Metric 1





Numerical Evaluation of Mutual Information

Optimal Parameter (5 min Window) Range Identification for Performance Below 5% Percentile

Parameter	Sampling Time	Range	Probability of Poor Performance
State Variable 1	188	[20, 30]	0.13
State Variable 2	392	[23, 27] and [47, 53]	0.14 and 0.17
State Variable 3	422	[25, 30] and [45, 50]	0.17 and 0.25
State Variable 4	227	[1.0, 1.1]	0.19
State Variable 5	**98**	[1.24, 1.26]	0.15
State Variable 6	167	0.1 and [100, 120]	**0.29 and 1**

Numerical Evaluation of Mutual Information

Optimal Parameter (30 min Window) Range Identification for Performance Below 5% Percentile

Parameter	Sampling Time	Range	Probability of Poor Performance
State Variable 1	128	[20, 30]	0.13
State Variable 2	83	[1.24, 1.26]	0.16
State Variable 3	55	[23, 26]	0.22
State Variable 4	**35**	[25, 29]	**0.25**
State Variable 5	363	[0.95, 1.15]	0.08
State Variable 6	355	[0, 75]	0.07

Numerical Evaluation of Mutual Information

Optimal Parameter (5 min Window) Joint Range Identification for Performance Below 5% Percentile

Parameter	Sampling Time	Range	Probability of Poor Performance
State Variable 1	59	[22, 28]	0.44
State Variable 2		[23, 26]	
State Variable 3		[25, 28]	

Parameter	Sampling Time	Range	Probability of Poor Performance
State Variable 1	145	[20, 30]	0.57
State Variable 2		[22, 24.5]	
State Variable 3		[23, 26]	
State Variable 4		[0.9, 1] and [1.2, 1.5]	
State Variable 5		[1.243, 1.263]	
State Variable 6		0.1	

Prediction of Yield/Ash

Regression Analysis

Bayesian Estimation Methods

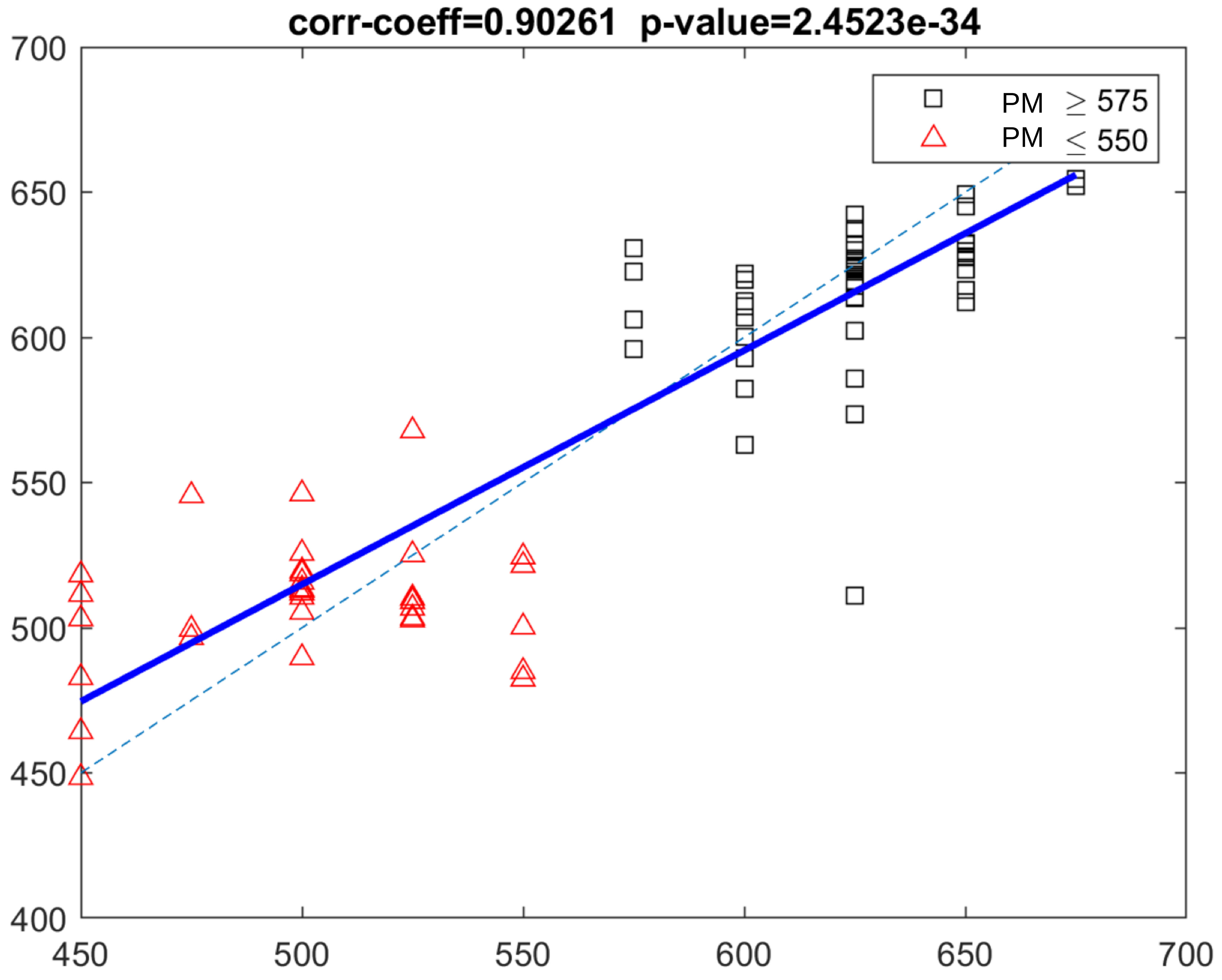
- We studied the feasibility of **Minimum Mean Square Error (MMSE)** estimators: not feasible at this stage due to lack of training data.
  - Second order statistics are required for time-series.
  - Mismatch introduced by **data scarcity** and **dynamics** of the time-series is too large.
  - Worth revisiting if there is more data available: **Kalman Filter** to exploit dynamical nature of data.

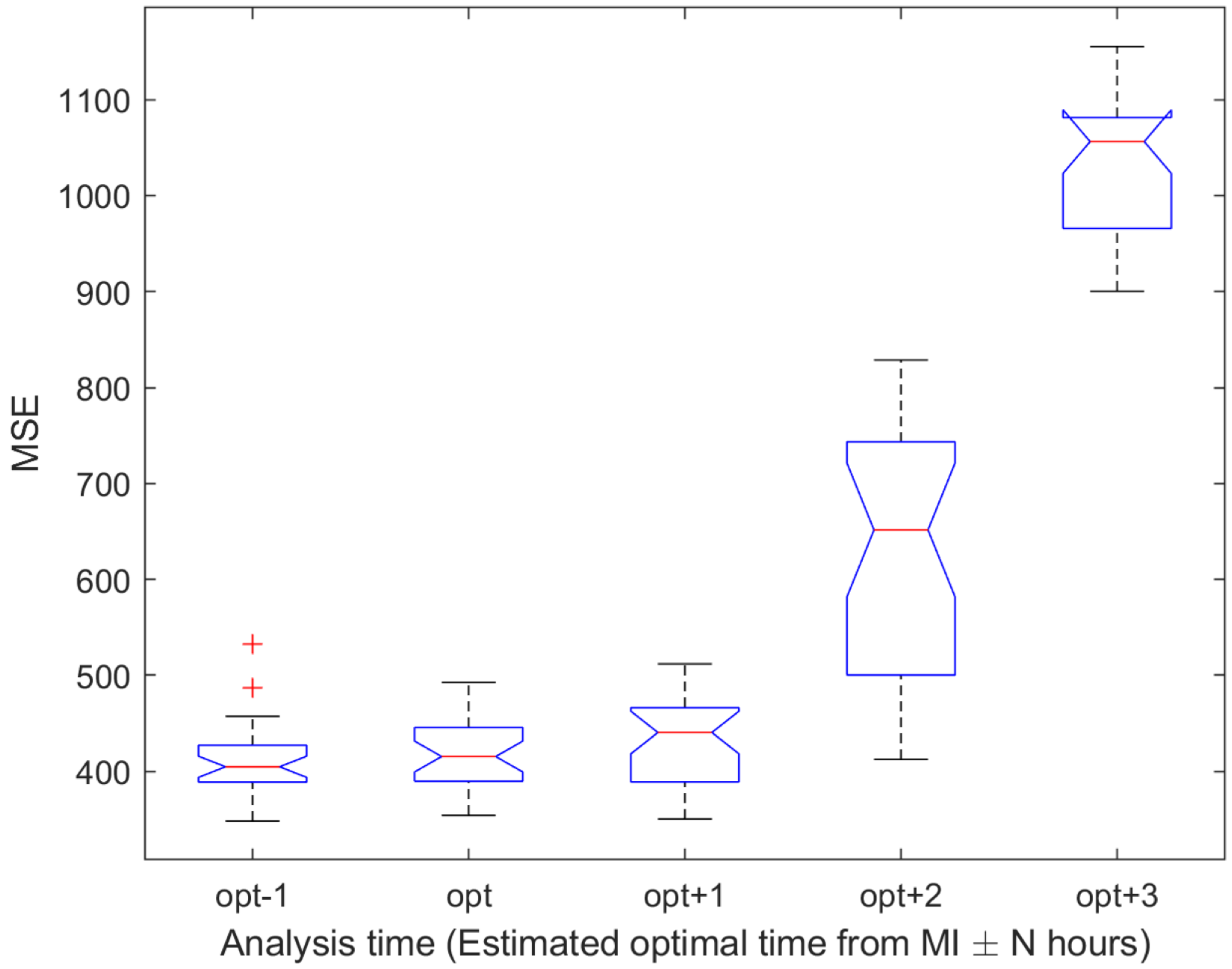
Neural Network based Regression

- Neural networks are **universal approximators.**
- Efficient learning paradigm that achieves good performance in several learning tasks.
- We cannot input the raw time-series to the neural network due to the lack of sufficient data.
- Current regression **error is moderate** but our simulations rely on synthetically generated data.
- Our data sampling method **improves performance** with respect to visually selected features.
  - Future exploitation of the data will benefit from mutual information based sampling.
  - More data required to characterize validity of neural networks for high-precision tasks.
- We plan to carry out uncertainty analysis to understand the effect of dynamics; possibly across multiple process stages.

Prediction of Performance Metric Forecasting

Numerical Results





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Information Measures based Regularization to Overcome Data Scarcity

S.M. Perlaza, G. Bisson, I. Esnaola, A. Jean-Marie, and S. Rini, "*Empirical Risk Minimization With Relative Entropy Regularization: Optimality and Sensitivity Analysis,"* in Proc. IEEE International Symposium on Information Theory, Helsinki, Finland, Jul. 2022

Problem Formulation: ERM with Relative Entropy Regularization (ERM-RER)

The ERM-RER problem, with parameters $Q \in \triangle(\mathcal{M}, \mathscr{B}(\mathcal{M}))$ and $\lambda \in (0, +\infty)$, consists of the optimization over the domain $\triangle_Q(\mathcal{M}, \mathscr{F}) \triangleq \{P \in \triangle(\mathcal{M}, \mathscr{F}) : P \ll Q\}$ given by

$$\min_{P \in \triangle_Q(\mathcal{M}, \mathscr{B}(\mathcal{M}))} \mathsf{R}_{\boldsymbol{z}}(P) + \lambda D(P \| Q).$$

Theorem

For all $\lambda \in \mathcal{K}_{Q,\boldsymbol{z}}$, the solution to the ERM-RER problem, denoted by $P^{(Q,\lambda)}_{\boldsymbol{\Theta}|\boldsymbol{Z}=\boldsymbol{z}} \in \triangle_Q(\mathcal{M}, \mathscr{B}(\mathcal{M}))$, is a **unique** *measure whose Radon-Nikodym derivative with respect to Q satisfies for all $\boldsymbol{\theta} \in \mathrm{supp}(\mathrm{Q})$,*

$$\frac{\mathrm{d}P^{(Q,\lambda)}_{\boldsymbol{\Theta}|\boldsymbol{Z}=\boldsymbol{z}}}{\mathrm{d}Q}(\boldsymbol{\theta}) = \exp\left(-K_{Q,\boldsymbol{z}}\left(-\frac{1}{\lambda}\right) - \frac{1}{\lambda}\mathsf{L}_{\boldsymbol{z}}(\boldsymbol{\theta})\right).$$

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Conclusions

1. Information Measures enable definition of a Quantitative Framework

- Information measures are **operationally meaningful** metrics
- Provide data acquisition system **design guidelines:** **optimal parameters** and **sampling times**
  - Simpler **digital infrastructure**
  - Sense only the informative data: **less sensors**
  - Save only the necessary data: **less data storage**

2. Feature Identification in Dynamic Multi-Stage Settings with Data Scarcity

- Systematic characterisation of relevant features
- Clustering and classification based on information density
- Fundamental limits describe best achievable performance

3. Novel information based regularization to leverage expert knowledge and first principles

- Mitigate data scarcity
- Provide explainability and robustness guarantees for ML tools

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Thanks!

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