Multi-Scale Uncertainty Analysis for Data Driven Models of Oxyfuel Combustion in Bubbling Fluidized Bed Combustor

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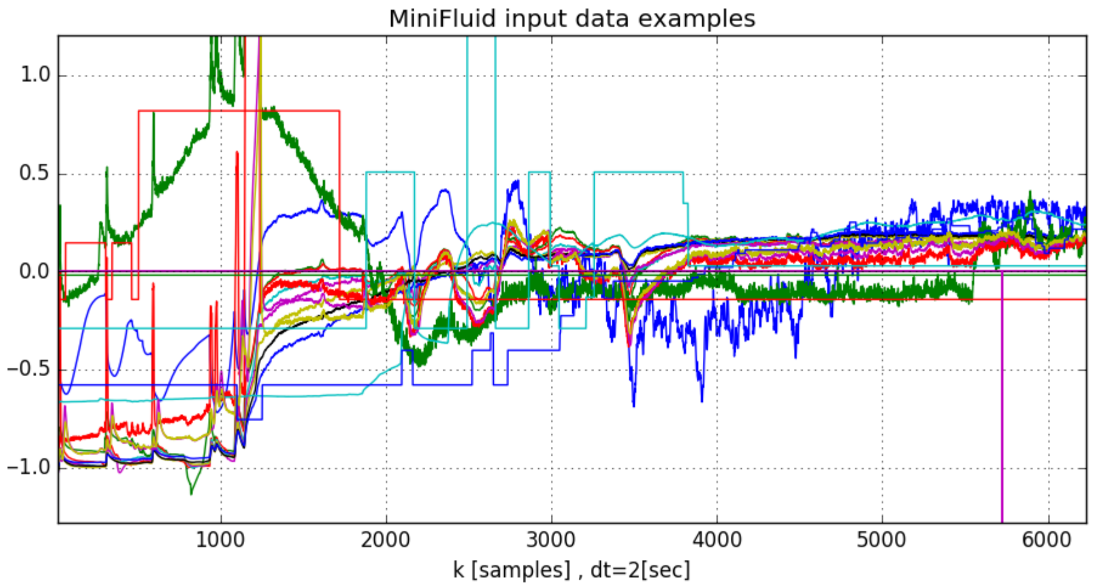
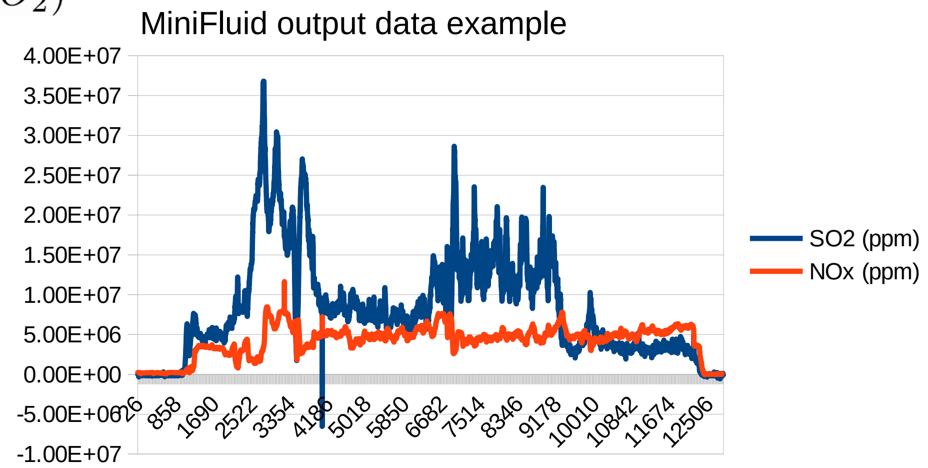
Motivation

- The oxyfuel combustion in a bubbling fluidized bed combustor is relatively new technology, and the combustion process is a complex nonstationary MIMO process:
  - about 33 input variables (incl. temperatures), and
  - at least 5 output variables $(CO_2, CO, SO_2, NO_x, O_2)$





We wish to developed reliable data-driven dynamical model of the oxyfuel combustion process, and proper (or mutliple validated) feature selection method is crucial esp. in case of system nonlinearity.

Motivation

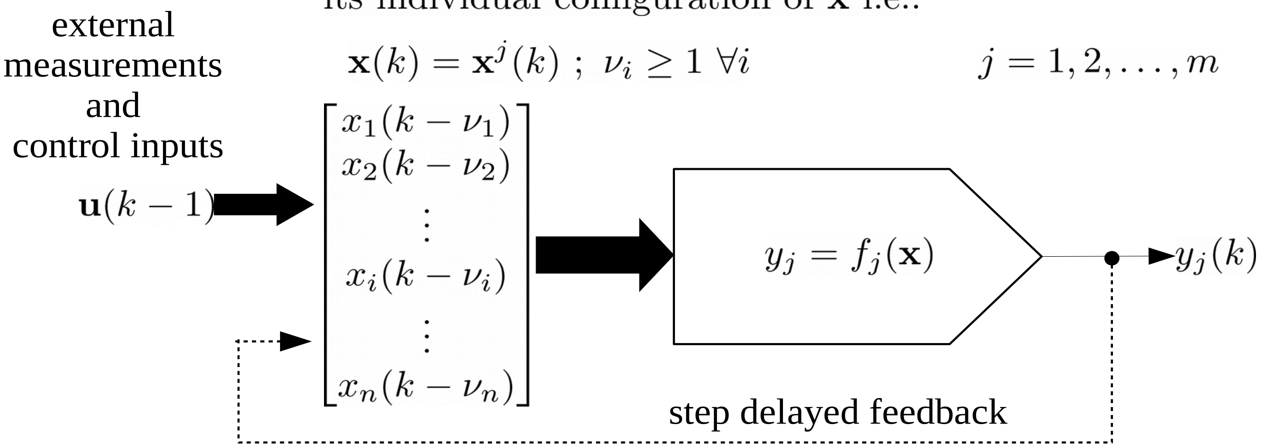
- The oxyfuel combustion in a bubbling fluidized bed combustor is relatively new technology, and the combustion process is a complex MIMO process:
  - about 33 input variables (incl. temperatures), and
  - at least 5 output variables $(CO_2, CO, SO_2, NO_x, O_2)$
- The accurate physical dynamical model of the process is unreachable and the process parameters (such as of the input fuel, etc) are not exactly known.
- We are researching the use of data-driven approaches (such as regression models, neural networks, Bayesian models, etc) to model the process with prospects of its optimization and control.
- Optimization techniques to achieve robust auto-regressive models are still a challenge.
- **At first here, we are focusing on data analysis for the feature vector of discrete-time dynamical computational models.**

Motivation

- A MIMO model can be implemented as multiple MISO models (multiple-input single output) $y_j = f_j(\mathbf{x}_j)$, where $f_j(.)$ denotes a computational model (regression model, neural network, Bayesian model) in general.
- It is easy to train a neural network to exactly fit the model for training data; however, this does not assure a correct model function for new input data (due to process nonlinearity, nonstatonarity, and variability in time <=> too many degrees of freedom)
- We need our computational model be causally correct, and it can hardly be achieved without a proper input data
- So the question is: **What is the proper configuration of input vector $\mathbf{x}$?** (i.e. What inputs and what feedbacks in $\mathbf{x}$? How long their history (how many step delays)?….)

each output variable y_j can have its individual configuration of $\mathbf{x}$ i.e.:

$$\mathbf{x}(k) = \mathbf{x}^j(k) \; ; \; \nu_i \geq 1 \; \forall i \qquad j = 1, 2, \ldots, m$$



Presentation Outline

- We will briefly discuss some fundamentals of methods for feature selection for data driven dynamical models (such as regression models, neural networks, Bayesian approaches,…) for complex multiple-input multiple-output (MIMO) systems
  - linear cross-correlations,
  - Principal Component Analysis (PCA),
  - neural network based auto-encoders,
  - Mutual Information (probability/likelihood) based techniques
- and then

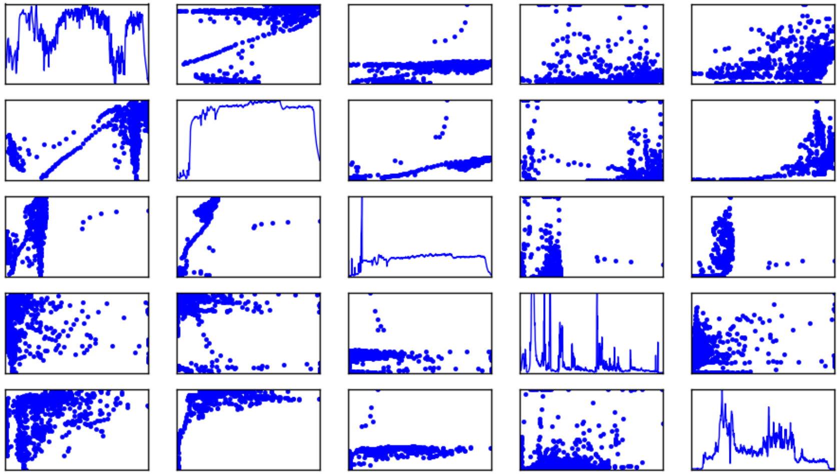
the presentation Objective

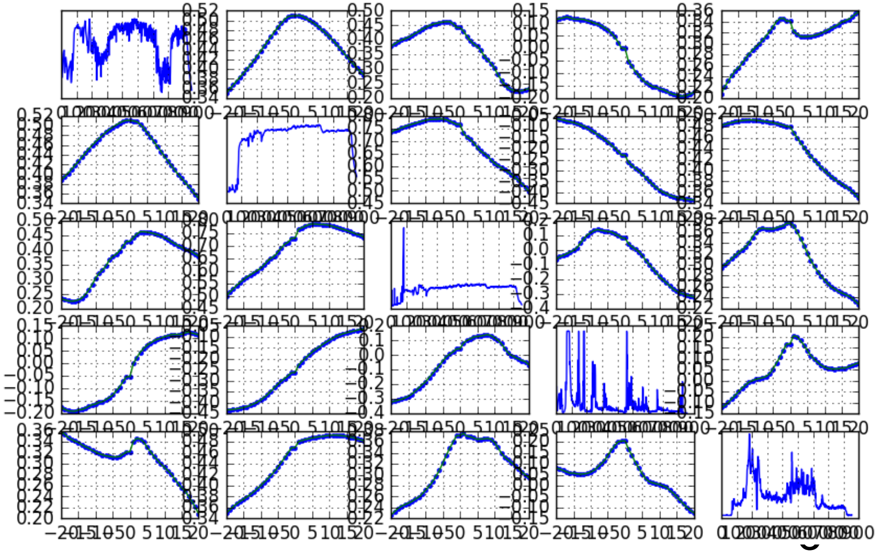
we discuss possible research direction of our original method [a] for
new research of feature selection via multi-scale false neighborhood minimization
(for optimizing the configuration of data driven discrete-time dynamical computational models)

[a] BUKOVSKY, I., Witold KINSNER, V. MALY a K. KREHLIK. Multiscale Analysis of False Neighbors for state space reconstruction of complicated systems. In 2011 IEEE Workshop On: Merging Fields of Computational Intelligence and Sensor Technology (CompSens) . 2011,p. 65–72. doi:10.1109/MFCIST.2011.5949517

Linear Cross-Correlation for MIMO Systems

- The cross correlation is for bi-variate linear dependency (SISO input-output), i.e., it evaluates the strength of linear relationship between two scalar variables.
- For MIMO systems it serves to reveal co-linearity among input variables.
- Assuming real processes are not so heavily nonlinear, the linear cross-correlation may be a first-to-do technique to:
  - indicate correlations of some input and output variables (if it can be linearly captured)
  - obtain some notion about time-shift (lag) between input and output variables
- However, for nonlinear MIMO systems, we can hardly use linear cross-correlation for more advanced model design

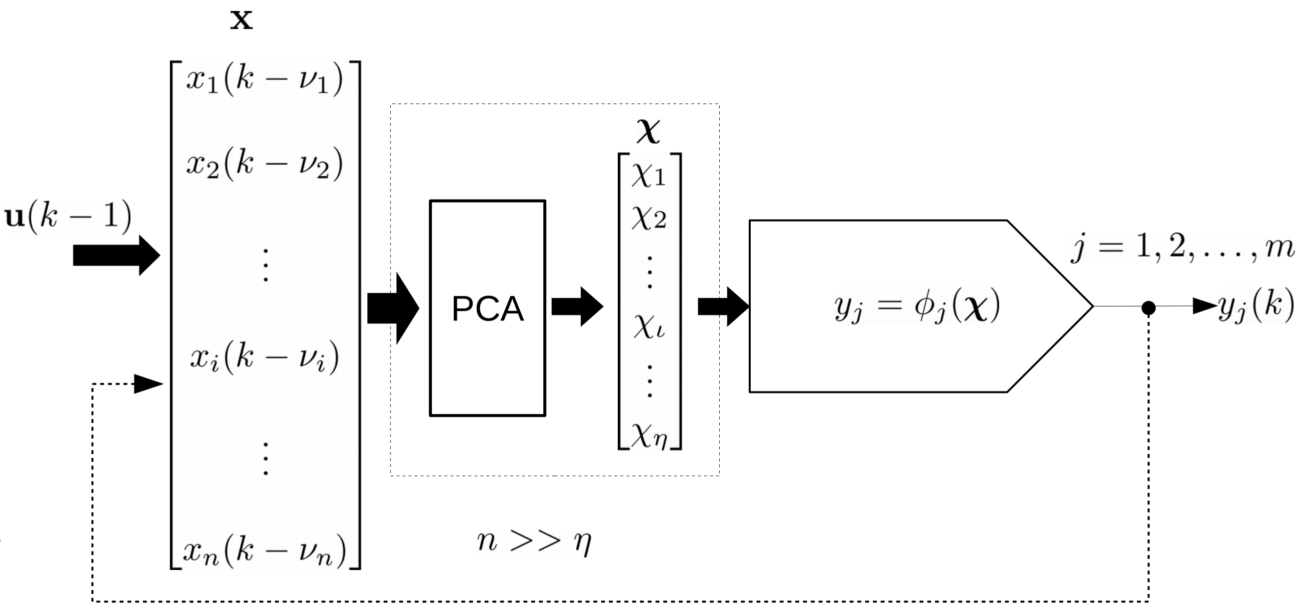




Principal Component Analysis (PCA) for (dynamical) Data Driven Models

- PCA is a classical linear transformation method that:
  - is based on linear cross-correlations, so
  - it reduces input data dimensionality via linear compression
    i.e. $\mathbf{X} \rightarrow \boldsymbol{\chi}$ (right fig.)

    while preserving the desired amount of information in data



- We applied PCA to dimensionality reduction for MIMO dynamical model of coal powder combustion process [b], where we decreased model complexity and suppressed outliers; however, the accuracy of the auto-regressive prediction was still limited (esp. for emissions of CO, CO_2)

- Furthermore, PCA as a dimensionality reduction technique is not suitable for direct feature selection (input $\mathbf{x}$ configuration, sensor selection), so additional techniques together with PCA has to be used.

[b] BUKOVSKÝ, Ivo a Michal KOLOVRATNÍK. A Neural Network Model for Predicting NOx at the Mělník 1. Acta Polytechnica [online]. 2012, 52(3) [vid. 2015-01-26]. ISSN 1805-2363. doi:10.14311/1538

Neural Network based Auto-Encoders for Data Driven Dynamical Models

- Auto-encoders (AE) are nonlinear mappings that encode (compress) and then decode (decompress) input data, so they perform nonlinear dimensionality reduction via some customized optimization algorithm.

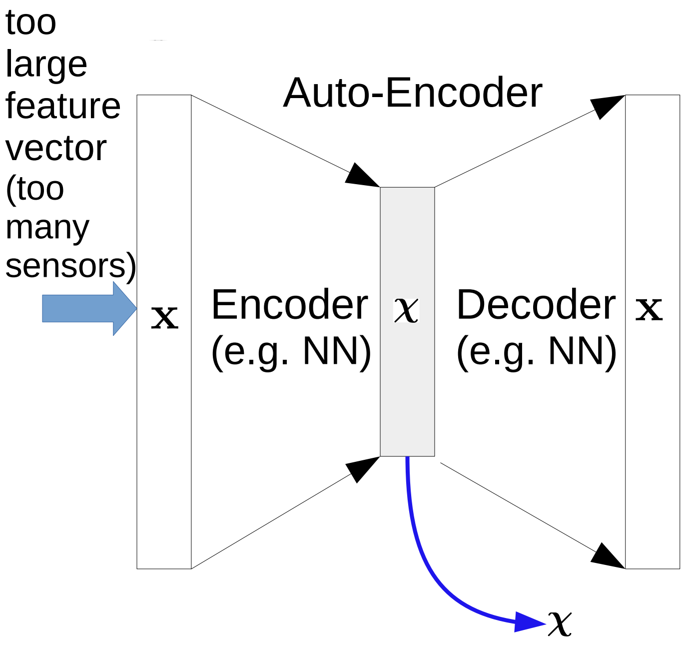
- AE has been widely studied and applied in Deep Learning that excels esp. in image and speech recognition nowadays.

- The application of Deep Learning in complicated tasks such as medical imaging or prediction of complex nonstationary dynamical MIMO systems is still an actual challenge.

- Because of customizable structure, the AE can combine linear and nonlinear dimensionality reduction.

- Extending studies of using AE for feature extraction for dynamical systems has been appearing in literature just since recently.

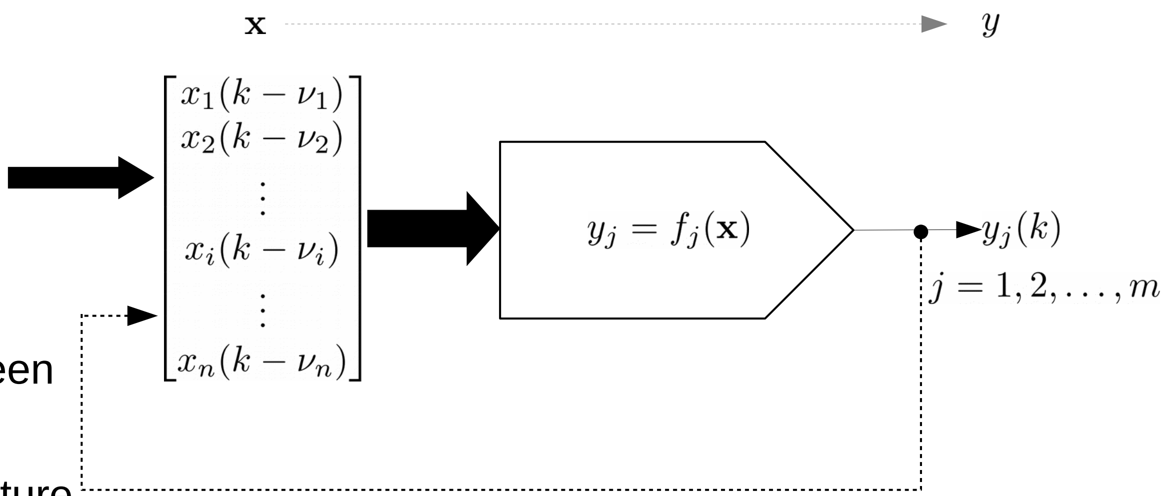
- The performance of AE can be excellent; however, it depends on:
  - their custom design,
  - selected (optimization) algorithms and its setups,
  - quality and amount of training data.



Mutual Information (probability/likelihood) Techniques for Data Driven Models

- Mutual Information (MI, Shannon 1948) is a probabilistic measure that quantifies the strength of nonlinear relationships.

$$MI(\mathbf{x}, y) = \sum_{y \in Y} \sum_{\mathbf{x} \in X} p(\mathbf{x}, y) \log \left(\frac{p(\mathbf{x}, y)}{p(\mathbf{x})\, p(y)} \right)$$



- Furthermore, MI can quantify the strength of nonlinear relationship not only between two scalar variables, but also between two vectors; thus,

- MI concept is more suitable for nonlinear feature selection, i.e. for configuration of input vector $\mathbf{x}$ via optimizing a suitable criterion Q that utilizes maximizing the strength of nonlinear relationship between $\mathbf{x}$ and y , i.e.

$$Q\Big(arg\big(max\{MI(\mathbf{x}, y)\}\big), \ldots\Big) \implies \mathbf{x}$$

- More recent achievements on information theoretic nonlinear feature selection via MI and recommendations on particular criteria selection and on suitability for small data set can be found in [c].

[c] Brown, G., Pocock, A., Zhao, M.J. and Luján, M. "Conditional Likelihood Maximisation: A Unifying Framework for Information Theoretic Feature Selection." Journal of Machine Learning Research 13 (2012): 27--66.

Here, finally the our method and its extension…

Multi-Scale Uncertainty Analysis for Data Driven Models...

- By the ***Uncertainty*** (in the design of input vector $\mathbf{x}$ for a given training data), we mean the existence of ***False Neighbors*** , i.e. if for two distinct times k_i , k_j:

$$\text{if } ||\mathbf{x}(k_i) - \mathbf{x}(k_j)|| < R_x \ AND \ ||y(k_i) - y(k_j)|| > R_y$$

$$\text{then } \mathbf{x}(k_i) \text{ and } \mathbf{x}(k_j) \text{ are false neighbors in } \mathbf{R}^n$$

- Nowadays, there exists published methods on feature selection via false neighborhood concept; however, usually with scalar thresholds Rx and Ry...
- We consider the user-defined fixed scalar thresholds Rx and Ry be still a challenge for further improvement of feature selection methods
- In [a] based on cumulative-sum approximation of power-law measure for multi-fractals, we have proposed to evaluate false neighbors in data over the whole range of setups of thresholds (to cope with the issue of a priory unknown optimal values of the thresholds Rx and Ry).
- Next slide recalls the core of this multi-scale method, and then the current research extension is presented

Multi-Scale False Neighborhood Analysis for Data Driven Models...

if $||\mathbf{x}(k_i) - \mathbf{x}(k_j)|| < R_x \; AND \; ||y(k_i) - y(k_j)|| > R_y$ then $\mathbf{x}(k_i)$ and $\mathbf{x}(k_j)$ are false neighbors in $\mathbf{R}^n$

- The method is based on cumulative-count approximation of power-law measure for multi-fractals ,
- so instead of detecting and counting False Neighbors (FN) for constant thresholds *Rx* and *Ry*,
- we detect and count FN for the range of thresholds $Rx=\{Rx_1,Rx_2,Rx_3,\ldots\}$, $Ry=\{Ry_1,Ry_2,Ry_3,\ldots\}$ via ***Areal Cumulative FN*** count or ***Diagonal Cumulative FN*** count as:

$$ACFN = \sum_{\forall i} \sum_{\forall j} FN(Rx_i, Ry_j) \qquad DCFN = \sum_{\forall i} FN(Rx_i, Ry_i)$$

where *FN*(.) is the count of false neighbors in the all dataset for given thresholds.

please see [a] for more details on *False Neighbor Matrix* and on power-law cumulative sum approximation.

- In the very principle, the above cumulative measures helps to avoid the risk of inappropriate threshold selection if FN shall be found via merely single valued thresholds *Rx* and *Ry*.
- The next slide shows (and discuss) ideas of our new research as we wish to developed fully automated multi-scale method for feature selection to achieve more reliable data driven model of the oxyfuel combustion process.

Multi-Scale False Neighborhood Analysis for Data Driven Models…
Current Research Extension

- We are developing a method that will design (or will be a supportive method for) the automated input vector configuration (feature selection) for complex data-driven dynamical MIMO model of (oxyfuel combustion) via the multi-scale false neighborhood concept ,i.e. via minimizing false neighbors in model configuration and its training data
- Currently several directions are investigated:

$$\begin{array}{ccccc} \boldsymbol{\theta} & & \mathbf{x} & & \\ \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_i \\ \vdots \\ \theta_n \end{bmatrix} & \times & \begin{bmatrix} x_1(k-\nu_1) \\ x_2(k-\nu_2) \\ \vdots \\ x_i(k-\nu_i) \\ \vdots \\ x_n(k-\nu_n) \end{bmatrix} & = \mathbf{x}_{\boldsymbol{\theta}} \end{array}$$

$$\theta_j = \begin{cases} 0 \ldots & \text{feature is not selected} \\ 1 \ldots & \text{feature is selected} \end{cases} \qquad \forall j$$

1) Being inspired by other feature optimization concepts, e.g. via the informatic theoretic feature selection [c] and optimization techniques therein, we may apply some optimization technique to a binary feature selection vector $\boldsymbol{\theta}$ (right top), so we can *search for minimum configuration of* $\mathbf{x}$ *with minimum number of multiscale false neighbors.*

2) The *sampling period of a model can be optimized via minimizing the multi-scale false neighbors*

3) Other optimization techniques to find a minimal input vector $\mathbf{x}$ with minimal multi-scale false neighbor measures … (?)

Summary

- We briefly reviewed some principles and discussed their potentials for feature selection for data-driven MIMO dynamical systems, i.e.:
  - Linear cross-corelations as the most fundamental method for getting first notion about possible relationships between data; however, that is rigorously unsuitable for design of nonlinear MIMO systems
  - PCA that reduces dimensionality of a feature vector; however, that is limited by its linearity and needs other extensions to perform feature extraction
  - Auto-encoders that perform powerful nonlinear dimensionality reduction; however, their use for nonlinear data-driven dynamical models, i.e. long term auto-regressive predictors is still not much explored
  - Information theoretic nonlinear feature selection, i.e. based on Mutual Information (probability/likelihood), as rather a well explored concept and popular domain
- Then, we recalled our original method on multiscale false neighbors analysis that is robust against the inappropriate threshold selection for false neighborhood, and
- we indicated its potentials for development of a new type of computationally effective automated feature selection method to support the design of complex data-driven dynamical systems.

- We hope, you could find something interesting in our presentation,
- we hope, we might initiate discussion and get your very valuable feedback (now or later)
- we hope, you are enjoying the Workshop and your stay in Prague

Thank you very much for your attention!!!

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