Control theoretically explainable application of autoencoder methods to fault detection in nonlinear dynamic systems

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Abstract

This paper is dedicated to control theoretically explainable application of autoencoders to optimal fault detection in nonlinear dynamic systems. Autoencoder-based learning is a standard machine learning method and widely applied for fault (anomaly) detection and classification. In the context of representation learning, the so-called latent (hidden) variable plays an important role towards an optimal fault detection. In ideal case, the latent variable should be a minimal sufficient statistic. The existing autoencoder-based fault detection schemes are mainly application-oriented, and few efforts have been devoted to optimal autoencoder-based fault detection and explainable applications. The main objective of our work is to establish a framework for learning autoencoder-based optimal fault detection in nonlinear dynamic systems. To this aim, a process model form for dynamic systems is firstly introduced with the aid of control theory, which also leads to a clear system interpretation of the latent variable. The major efforts are made on the development of a control theoretic solution to the optimal fault detection problem, in which an analog concept to minimal sufficient statistic, the so-called lossless information compression, is introduced and proven for dynamic systems and fault detection specifications. In particular, the existence conditions for such a latent variable are derived, based on which a loss function and further a learning algorithm are developed. This learning algorithm enables optimally training of autoencoders to achieve an optimal fault detection in nonlinear dynamic systems. A case study on three-tank system is given at the end of this paper to illustrate the capability of the proposed autoencoder-based fault detection and to explain the essential role of the latent variable in the proposed fault detection system.

Key words: Fault detection; autoencoder; system image representation; lossless information compression; minimal sufficient statistic

1 Introduction

Associated with increasing demands on production efficiency and system performance, today’s industrial processes are of an extremely high degree of complexity and nonlinearity. For such type of systems, safety and reliability are of significant importance, which motivates the development of fault detection methods (Blanke et al., 2006; Ding, 2008). Reviewing the publications on fault detection in nonlinear control systems shows that the observer-based schemes serve as a major methodology (Tan & Edwards, 2002; Yang et al., 2015; Li et al., 2017a, b), and promise reliable fault detection. The application of the observer-based fault detection schemes requires a precise physical model of the system under consideration, which demands for considerable modeling efforts and, in turn, leads to high engineering costs. This calls for research endeavor to develop data-driven fault detection approaches (Ding, 2014). Among the involved studies, the subspace methods and multivariable statistic analysis build the main research stream (Huang & Kadali, 2008; Yang et al., 2015; Li et al., 2017a, b).
Nevertheless, these methods are incapable to handle highly nonlinear dynamics and thus mainly limited to linear or linearized systems.

In recent years, machine learning (ML) based methods have drawn remarkably increasing attention in both academic and industrial fields thanks to the learning capacity and the ability in dealing with nonlinearities by means of huge amount of process data (Haykin 2009). One of the most popular application areas of ML methods is classification, to which fault detection (also known as anomaly detection), as a typical one-class classification problem, belongs. Towards this end, intensive research efforts have been made in representation learning (Bengio et al. 2013). Roughly speaking, the basic idea behind ML-based fault detection methods lies in the reconstruction of process variables in the nominal process operation state. Different from the model- and observer-based methods, the ML-based reconstruction of the process variables under consideration is achieved by processing the process data collected and recorded during fault-free process operations, known as learning. Unfortunately, the learning capability often suffers considerably from uncertainties in the collected process data, like disturbances or variations caused by agings in assets. The so-called autoencoder (AE) method, an efficient ML-based tool for dimensionality reduction and feature learning, offers a reasonable and convincing solution to this problem (Hinton & Salakhutdinov 2006, Goodfellow et al. 2016). An autoencoder consists of an encoder that compresses the process data into the so-called latent (hidden) variable, and a decoder that is driven by the latent variable and reconstructs the process variables reflecting nominal process operations (Shao et al., 2021). Using neural networks (NNs), the encoder and decoder are learnt, in optimal case, in such a way that the latent variable contains exclusive informations (features) of the nominal process operations, from which the process variables in the nominal state are then fully reconstructed. The challenging issue in this learning process is how to learn such an (ideal) latent variable. In (Tishby & Zhangvalsky, 2015), the concept of information bottleneck has been introduced, which suggests that all the information from the input variables required in the reconstructing (estimating) target should be contained in the learned latent representation in the neural networks. In the information theoretical framework, (Tishby & Zhangvalsky, 2015, Geiger 2021) have proposed to generate latent variable as the so-called minimal sufficient statistic. On the basis of these concepts, the information plane analysis has been popularized by Shwartz-Ziv and Tishby, which showcases the important role of determining the latent representations aiming at high ML performance (Shwartz-Ziv & Tishby 2017). The methods of information plane analysis have been applied to construction of autoencoders as well (Yu & Principi, 2019, Tapia & Estevez, 2020).

A review of the existing AE-based fault diagnosis schemes gives the impression that the main focus of the reported efforts has been on a direct (and successful) application of the existing AE-algorithms and schemes to dealing with fault diagnosis issues (Jiang et al., 2017, Ahmed et al., 2022, Hu et al., 2022, Liu et al., 2021, Ren et al., 2020). In this regard, the latent variable is generally viewed as features generated by the learning process, without explainable interpretation and assessment of the (generated) latent variable with respect to its information quality, e.g. measured as minimal sufficient statistic. The consequence of such application-oriented research efforts is that there is a lack of a methodical framework for explainable applications of AE-based technique to approach optimal fault detection issues.

A further noteworthy aspect is that few of the existing AE-based fault detection schemes have been devoted to dynamic systems, as they are known in control theory and exist widely in industry. Moreover, existing control and system theoretic knowledge has been rarely utilized in those AE-based fault detection schemes. It should be noticed that the dynamic systems considered in our work differ from those typical objects and processes addressed by the existing AE-based methods generally in

• their complex dynamics,
  
  They are not only time evolutionary processes, but also driven by process input variables, which are operation condition triggered, strongly time-varying and often in feedback closed-loop configurations;

• existence of hybrid uncertainties,
  
  Typical uncertainties in industrial automatic control systems are disturbances, including (external) unknown inputs, process and measurement noises, variations in the environment around the process and within the process e.g. caused by agings in the operational and control assets, mismatching of embedded control loops, as well as errors generated during data transmissions among the subsystems over networks.

Although most of the existing observer-based fault detection methods successfully developed in the past decades (Tan & Edwards, 2002, Zhang et al., 2010, Yang et al., 2015, Li et al., 2017a,b) cannot be, due to the lack of process models, applied to realize data-driven fault detection, existing knowledge and ideas would be helpful to develop capable AE-based methods to approach optimal fault detection in nonlinear dynamic systems.

Motivated by the above discussions and observations, this paper is devoted to the research effort of control theoretically guided application of AE-based methods to approaching optimal fault detection in nonlinear dynamic systems. The main objectives and the intended contributions are
• introduction of a process model form for dynamic systems;
  This process model matches the configuration of an autoencoder with a clear interpretation of the latent variable. To this aim, the so-called coprime factorization technique will serve as a tool, and the concepts of system image representation and subspace are introduced.
• development of a control theoretic solution to optimal fault detection;
  The centerpiece of this solution is the introduction of an analog concept to minimal sufficient statistic for nonlinear dynamic systems and learning of the latent variable. In particular, the existence conditions for such a latent variable will be derived. Based on image representation and subspace of nonlinear systems, methods of Hamiltonian extension and analysis of inner systems will be applied.
• information theoretic study on the proposed latent variable;
  On assumption of a defined probabilistic setting and using the concept of mutual information, it is proven that the proposed latent variable is equivalent to a minimal sufficient statistic.
• construction of an autoencoder;
  With the aid of the control theoretic results as guidelines, an autoencoder will be learnt that delivers a data-driven solution of the optimal fault detection problem for nonlinear dynamic systems. The core of this work is to recast the existence condition of the optimal latent variable as regularized terms in the loss function for learning the autoencoder.
• realization of the autoencoder and test on an experimental system, analysis of the fault detection performance of the developed autoencoder and the role of the latent variable in approaching the optimal solution.

The paper is organized as follows. The preliminaries and problem formulation are given in Section 2. Section 3 includes the main results and consists of four parts, (i) the basic ideas and optimal solution illustrated by means of linear systems and the associated concepts, (ii) the proof that the proposed latent variable is, in the context of mutual information, equivalent to a minimal sufficient statistic, (iii) the optimal solution for fault detection in nonlinear systems, and (iv) realization and implementation of the optimal solution by means of an autoencoder. Finally, in Section 4, the results on a case study on the laboratory setup of a three-tank system are presented and analyzed.

**Notations:** Throughout this paper, standard notations known in control theory, and in linear algebra are adopted. In addition, $T^\ast(s) = T^T(\ast s)$ (respectively $T^\ast(z) = T^T(z^{-1})$, $T^\ast(e^{\eta j\theta}) = T^T(e^{-\eta j\theta}) := T^T(-\theta)$) denotes the conjugate of (rational) transfer function matrix $T(s)$ (respectively $T(z), T(e^{j\theta}) = T(z)|_{z = e^{j\theta}} := T(\theta)$), and $L_2$ is the notation of the space of all square summable/integrable Lebesgue signals (signals with bounded energy) [Francis 1987; Vinnicombe 2000].

## 2 Preliminaries and problem formulation

### 2.1 Basics of data-driven fault detection paradigm for dynamic systems

Consider a nonlinear process $\Sigma : L_2 \rightarrow L_2$, whose nominal dynamic is modelled by

$$\Sigma : \begin{cases} \dot{x}(t) = f(x(t), u(t)) \\ y(t) = c(x(t), u(t)) \end{cases} \quad (1)$$

Here, $u \in \mathbb{R}^p, y \in \mathbb{R}^m, x \in \mathbb{R}^n$ denote the process input, output and state vectors, respectively. $f(\cdot)$ and $c(\cdot)$ represent nonlinear continuous functions. Taking into account possible disturbances in the process dynamic and measurement variables, the above model is extended to

$$\Sigma : \begin{cases} \dot{x}(t) = f(x(t), u(t), \eta(t)) \\ y(t) = c(x(t), u(t), \varepsilon(t)) \end{cases} \quad (2)$$

where $\eta, \varepsilon$ represent unknown and $L_2$-bounded signals. $f(\cdot)$ and $c(\cdot)$ denote nonlinear continuous functions. Model (2) represents the process dynamics during fault-free operations.

As often met in industrial applications, it is supposed, in our subsequent study, that

- the model (2) is unknown, and instead,
- sufficient process data, $(u, y)$, are collected and recorded during fault-free operations, and
- they are available for the purpose of learning process dynamics during fault-free operations.

The major task of designing and operating a fault detection system is to detect process operations that lead to a significant deviation of process performance from its nominal value. It is a well-established paradigm of approaching data-driven fault detection in dynamic systems with the following steps and specifications:

- learn a dynamic system II using the collected fault-free process data. II is driven by process data $(u, y)$ and delivers $(\hat{u}, \hat{y})$ serving as an estimate for the process input and output variables in the nominal operations, i.e.

$$\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} := \Pi \begin{bmatrix} u \\ y \end{bmatrix}$$

- learning II should satisfy, at a high probability, the specifications that (i) for data $(u, y)$ generated during fault-free operations,

$$\left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|^2 \leq J_{th}, \quad (4)$$

$$\left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|^2 \leq J_{th}, \quad (4)$$
AE-based fault detection is one of numerous application areas of AE methods and attracts increasing attention in recent years (Jiang et al., 2017; Ahmed et al., 2022; Hu et al., 2022; Liu et al., 2021; Ren et al., 2020; Yan et al., 2021; Tang et al., 2021; Zhao et al., 2020). The basic idea behind the AE-based fault detection lies in the reconstruction of process variables corresponding to nominal process operations. To this aim, an autoencoder is learnt using process operation data collected during fault-free operations. An AE is composed of two system parts, an encoder that compresses the process variables into a (low-dimensional) latent variable, and a decoder that reconstructs the process variables from the latent variable. To be specific, consider a process described by $\Sigma$ with process input and output variables $(u,y)$. Using neural networks, $\mathcal{N}\mathcal{N}_{en}$ and $\mathcal{N}\mathcal{N}_{de}$ with $\theta_{en}, \theta_{de}$ as the associated parameters, the encoder and decoder are constructed as follows:

$$v = \mathcal{N}\mathcal{N}_{en}(\theta_{en}, [u, \hat{y}]) = \mathcal{N}\mathcal{N}_{de}(\theta_{de}, v) \implies$$

$$\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = \mathcal{N}\mathcal{N}_{de}(\theta_{de}, \mathcal{N}\mathcal{N}_{en}(\theta_{en}, [u, y])). \quad (6)$$

where $v$ is the latent variable and $\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix}$ denotes the reconstructed process variables that should reflect the nominal process operations. Fig. 2 showcases the structure of an AE.

To learn an AE, a standard and basic loss function is the squared reconstruction error, for instance, defined by

$$\mathcal{L}(\theta_{de}, \theta_{en}) = \frac{1}{M} \sum_{i=1}^{M} \left[ \begin{bmatrix} u(i) \\ y(i) \end{bmatrix} - \begin{bmatrix} \hat{u}(i) \\ \hat{y}(i) \end{bmatrix} \right]^T \left[ \begin{bmatrix} u(i) \\ y(i) \end{bmatrix} - \begin{bmatrix} \hat{u}(i) \\ \hat{y}(i) \end{bmatrix} \right],$$

$$\begin{bmatrix} \hat{u}(i) \\ \hat{y}(i) \end{bmatrix} = \mathcal{N}\mathcal{N}_{de}(\theta_{de}, \mathcal{N}\mathcal{N}_{en}(\theta_{en}, [u(i), y(i)])).$$

Here, $\begin{bmatrix} u(i) \\ y(i) \end{bmatrix}$ represents a data sample (or batch) from the data set, and $M$ denotes the number of the data samples (batches) used for the learning purpose. The parameters $\theta_{en}, \theta_{de}$ are to be determined by solving the optimization problem

$$\min_{\theta_{en}, \theta_{de}} \mathcal{L}(\theta_{de}, \theta_{en}).$$

For the fault detection purpose, it is natural to use the trained autoencoder (i) to generate

$$\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = \mathcal{N}\mathcal{N}_{de}(\theta_{de}, \mathcal{N}\mathcal{N}_{en}(\theta_{en}, [u, y])).$$

hereby, signal vector

$$r := \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \in \mathbb{R}^{p+m}$$

is often called residual (vector), (ii) in case of $(u, y)$ being generated by a faulty operation,

$$||r||^2 > J_{th},$$

where $\|\cdot\|$ denotes a certain signal norm;

• as a part of the learning process, the so-called threshold $J_{th}$ should be determined so that the following detection logic holds

$$\left\{ \begin{array}{l} ||r||^2 \leq J_{th}, \text{ during fault-free operations} \\ ||r||^2 > J_{th}, \text{ in case of faulty operations.} \end{array} \right. \quad (5)$$

Fig. 1 schematically sketches the configuration and composition of such a fault detection system.

In engineering practice, the fault detection performance is mainly assessed by the fault detectability subject to a user-defined upper bound of a false alarm rate (FAR). Both in research and application domains, the fault detectability and false alarm rate are often expressed by the probability of successful detection of faulty operations and the probability of (false) alarms in fault-free operations, respectively (Ding, 2008). In this regard, data-driven design of an optimal fault detection system is formulated as: given sufficient process data $(u, y)$ collected during fault-free operations and the evaluation function $||r||^2$, finding $(\Pi, J_{th})$ so that the fault detectability is maximized while satisfying the user-defined FAR requirement.

2.2 Basics of autoencoder technique and its applications to fault detection

Autoencoder methods are a well-established technique in ML (Hinton & Salakhutdinov, 2006; Goodfellow et al., 2016). AE-based fault detection is one of numerous
Fig. 2. The schematic of an autoencoder using online data $\begin{bmatrix} u \\ y \end{bmatrix}$, (ii) to run the evaluation function

$$J = \left( \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right)^T \left( \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right),$$

and finally (iii) to make a decision according to the detection logic

$$\begin{array}{l}
J > J_{th} \implies \text{faulty} \\
J \leq J_{th} \implies \text{fault-free},
\end{array}$$

where the threshold $J_{th}$ is set by means of the (minimum) value of the loss function delivered by training.

2.3 Problem formulation

It is a widely recognized and accepted fact that, thanks to the power of neural networks (including deep NNs) of approximating nonlinear functions and systems, an autoencoder delivers optimal reconstruction of process variables with respect to the defined loss function. For instance, when a static (and statistic) process is under consideration, it has been proven that an autoencoder with the squared reconstruction error as the loss function is equivalent to the well-known principle component analysis (PCA) algorithm, which is widely applied in fault detection and process monitoring as well. Recently, efforts have been reported on improving fault detection performance by introducing regularized terms into the loss function to regularize the latent variable (Yan et al. 2021; Tang et al. 2021; Zhao et al. 2020).

Comparing the optimal fault detection problem formulated in Subsection 2.1 and the basic principle of the AE-based fault detection technique introduced in Subsection 2.2 leads to a convincing conclusion that the AE technique offers an efficient tool to solve the formulated optimal fault detection problem. On the other hand, to our best knowledge, no research work and results have been reported on such a solution. To approach the optimal solution, a challenging issue is how and to which degree the nominal process operations can be fully reconstructed by means of the process data, collected during fault-free operations but corrupted with noises or operation uncertainties. In fact, this is the major concerning of observer-based fault detection technique as well, which, as a special form of the fault detection system (3)-(4), is based on the reconstruction of the process output variable using a nominal process model and thus considerably suffers from uncertainties. In the ML framework, this problem is reflected in a different form. Due to the capability of neural networks to approximate nonlinear functions, overfitting often leads to lower fault detectability, since uncertain operations would be learnt as a part of the system dynamics. This issue has been addressed in the context of the so-called information bottleneck (Bengio et al. 2013; Geiger 2021), which is expressed in form of latent variables. An ideal latent variable should be generated by maximally compressed mapping of the input variable that preserves as much as possible the information on the output variable, according to Tishby & Zaslavsky (2015). In the information theoretic framework, Tishby & Zaslavsky (2015); Geiger (2021) have proposed the concept minimal sufficient statistic, and suggested to optimize autoencoders by generating the latent variable in the sense of minimal sufficient statistic.

Motivated and inspired by the aforementioned discussions, the following problems and tasks are formulated for our subsequent study:

- establishing a framework for the reconstruction of nominal process variables $(u, y)$ on the basis of a latent variable. For this purpose, the so-called system coprime factorization technique, that is widely applied in observer-based fault diagnosis technique (Ding 2020), will serve as a tool;
- developing a control theoretic concept analog to minimal sufficient statistic, which allows a maximal compression of information in the process data $(u, y)$ about process nominal operations in terms of the latent variable and leads to a reconstruction of the nominal operations without loss of information. Control theoretic and mathematical existence conditions
for such a latent variable should be found;

- studying on a probabilistic interpretation of the latent variable as a minimal sufficient statistic with the aid of the established mutual information concept;
- constructing and learning autoencoders guided by the derived existence conditions, which should result in an AE-based solution of the formulated optimal fault detection problem, and finally,
- verifying the proposed AE-based optimal fault detection system and, in comparison with the standard AE-based schemes, analyzing the fault detection capability.

3 Main results

This section is devoted to a control theoretically guided learning of autoencoders aiming at optimally detecting faults in nonlinear dynamic systems. To this end, we first introduce and illustrate the basic idea in the well-established framework of linear system theory as well as its information theoretic interpretation. It is followed by a study on the extension of the basic idea to nonlinear dynamic systems, and finally its autoencoder-based realization.

3.1 Introduction of the basic idea

Consider a linear time invariant (LTI) system modelled by a transfer function matrix \( G(s) \), whose minimal state space representation is given by

\[
G : \begin{cases}
\dot{x}(t) = Ax(t) + Bu(t) \\
y(t) = Cx(t) + Du(t),
\end{cases}
\]

where \( A, B, C, D \) are system matrices of appropriate dimensions. A right coprime factorization (RCF) of \( G \) is given by \( G(s) = N(s)M^{-1}(s) \) with the right coprime pair \((M(s), N(s))\). The RCF of \( G \) can be interpreted as a state feedback control system with the closed-loop dynamics

\[
\begin{aligned}
\dot{x}(t) &= (A + BF)x(t) + BVv(t) \\
u(t) &= Fx(t) + Vv(t) \\
y(t) &= (C + DF)x(t) + DVv(t),
\end{aligned}
\]

where \( F \) as the state feedback gain is selected such that \( A + BF \) is Hurwitz, \( V \) as a pre-filter is an invertible constant matrix, and \( v \) serves as a reference signal. Correspondingly, \( M(s), N(s) \) are stable systems with the state space representations

\[
\begin{aligned}
M(s) &= (A + BF, BV, F, V), \\
N(s) &= (A + BF, BV, C + DF, DV).
\end{aligned}
\]

The system (7) is called stable image representation (SIR) of \( G \) and expressed in the frequency domain as

\[
I_G(s) : \begin{bmatrix} u(s) \\ y(s) \end{bmatrix} = \begin{bmatrix} M(s) \\ N(s) \end{bmatrix} v(s). \tag{10}
\]

Note that the SIR of \( G \) implies the input-output dynamic \( y = Gu \), i.e.

\[
y(s) = N(s)v(s), \quad v(s) = M^{-1}(s)u(s) \\
\Rightarrow y(s) = N(s)M^{-1}(s)u(s) = G(s)u(s).
\]

In this context, vector \( v \) acts as a latent variable.

**Remark 1** Hereafter, we may drop out the domain \( s \) or \( t \) when there is no risk of confusion.

During normal process operations, the process data \((u,y)\) build a subspace in the Hilbert space \( L_2 \), the so-called image subspace of \( G \), which is explicitly defined by the SIR of \( G \) and the latent variable \( v \) as follows

\[
\mathcal{L}_G = \left\{ \begin{bmatrix} u \\ y \end{bmatrix} : \begin{bmatrix} u \\ y \end{bmatrix} = \begin{bmatrix} M \\ N \end{bmatrix} v, v \in L_2 \right\}. \tag{11}
\]

It is of interest to notice that the nominal process data \((u,y)\) can be viewed as being generated by the latent variable \( v \) serving as an information signal (like the reference signal in a feedback control loop).

Now, we are in a position to introduce the basic idea of approaching the problem of designing optimal fault detection systems formulated in the previous section. Let \( \mathcal{P}_V \) be an operator defined on a subspace \( V \) in Hilbert space that is endowed with the inner product,

\[
\langle \alpha, \beta \rangle = \int_{-\infty}^{\infty} \alpha^T(t)\beta(t)dt, \alpha, \beta \in V \subset L_2.
\]

If \( \mathcal{P}_V \) is idempotent and self-adjoint, namely

\[
\forall \alpha, \beta \in V, \mathcal{P}_V^2 = \mathcal{P}_V, \langle \mathcal{P}_V\alpha, \beta \rangle = \langle \alpha, \mathcal{P}_V\beta \rangle, \tag{12}
\]

it is an operator of an orthogonal projection onto \( V \) \cite{Kato1995}. The following properties of an orthogonal projection are of importance for our solution \cite{Kato1995}:

- \( \forall \alpha \in V, \mathcal{P}_V\alpha = \alpha \iff \langle \mathcal{P}_V\alpha, \alpha - \mathcal{P}_V\alpha \rangle = 0; \)
- \( \forall \alpha \in L_2, \alpha = \mathcal{P}_V\alpha + \mathcal{P}_{V^\perp}\alpha, \) where \( V^\perp \) is the orthogonal complement of \( V; \)
- given \( \beta \in L_2, \forall x \in V \subset L_2, \)

\[
\langle \beta - \alpha, \beta - \alpha \rangle = \|\beta - \alpha\|_2^2 \geq \|\beta - \mathcal{P}_V\beta\|_2^2.
\]
Moreover, if the subspace \( V \) is closed, the distance between \( \beta \) and \( V \), \( \text{dist}(\beta,V) \), is defined as
\[
\text{dist}(\beta,V) = \inf_{\alpha \in V} \| \beta - \alpha \|_2, \tag{13}
\]
which can be computed as
\[
\text{dist}(\beta,V) = \| \beta - \mathcal{P}_V \beta \|_2 = \| \mathcal{P}_{V^\perp} \beta \|_2.
\]
It is well-known that the image subspace \( \mathcal{I}_G \) is closed in \( \mathcal{L}_2 \) and
\[
\Pi(s) = I_G(s) \tilde{I}_G(s),
\]
forms an orthogonal projection onto \( \mathcal{I}_G \) \cite{Vinnicombe2000}, denoted by \( \mathcal{P}_I \), namely
\[
\mathcal{P}_I \begin{bmatrix} u \\ y \end{bmatrix} = \Pi \begin{bmatrix} u \\ y \end{bmatrix} = I_{G,0}I_{G,0}^\perp \begin{bmatrix} u \\ y \end{bmatrix}. \tag{14}
\]
Here, \( I_{G,0} \) is the normalized SIR of \( G \) and satisfies
\[
I_{G,0}^\perp I_{G,0}(s) = M_0^\perp(s)M_0(s) + N_0^\perp(s)N_0(s) = I. \tag{15}
\]
The pair \((M_0,N_0)\) is a RCF of \( G \) with the following setting for \( F,V \) given in (8)-(9) \cite{Hoffmann1996},
\[
F = -(I + DT^T)(DTC + B^TP),
\]
\[
V = (I + DT^T)^{-1/2},
\]
where \( P > 0 \) is the solution to the following Riccati equation
\[
A^TP + PA + C^TC - (D^TC + B^TP)^T R^{-1} (DTC + B^TP) = 0, \tag{16}
\]
where
\[
R = I + DT^TD.
\]
Note that operator \( I - \mathcal{P}_I : \mathcal{L}_2 \to \mathcal{L}_2 \),
\[
(I - \mathcal{P}_I) \begin{bmatrix} u \\ y \end{bmatrix} = (I - I_{G,0}I_{G,0}^\perp) \begin{bmatrix} u \\ y \end{bmatrix},
\]
defines an orthogonal projection onto the orthogonal complement of \( \mathcal{I}_G \), denoted by \( \mathcal{I}_G^\perp \). Consequently, any process data can be written as
\[
\begin{bmatrix} u \\ y \end{bmatrix} = \mathcal{P}_I \begin{bmatrix} u \\ y \end{bmatrix} + \mathcal{P}_{I_G^\perp} \begin{bmatrix} u \\ y \end{bmatrix}, \mathcal{P}_{I_G^\perp} = I - \mathcal{P}_I.
\]
In the context of one-class classification, faulty operations are detected if
\[
\begin{bmatrix} u \\ y \end{bmatrix} \notin \mathcal{I}_G \Rightarrow \mathcal{P}_{I_G^\perp} \begin{bmatrix} u \\ y \end{bmatrix} \neq 0,
\]
and \( \mathcal{P}_{I_G^\perp} \begin{bmatrix} u \\ y \end{bmatrix} \) is sufficiently large (with respect to a defined threshold, see below). In other words, in order to achieve a reliable and optimal fault detection, the test statistic or the residual evaluation function should be maximally sensitive to \( \mathcal{P}_{I_G^\perp} \begin{bmatrix} u \\ y \end{bmatrix} \). In order to gain a deeper insight into the concepts concerning \( \mathcal{I}_G, \mathcal{I}_G^\perp \) and normalized coprime factorizations, which are useful in our subsequent work, we briefly introduce some essential relations.

As the dual concepts to RCF and SIR, the so-called left coprime factorisation (LCF) and stable kernel representation (SKR) of \( G \) are well-established in factorization technique \cite{Vidyasagar1985, Vinnicombe2000}. Denoted by
\[
K_G(s) = \begin{bmatrix} -\tilde{N}(s) & \hat{M}(s) \end{bmatrix}
\]
with \( \hat{M}, \tilde{N} \) as a left coprime pair, the SKR \( K_G \) satisfies
\[
\begin{bmatrix} -\tilde{N}(s) & \hat{M}(s) \end{bmatrix} \begin{bmatrix} M(s) \\ N(s) \end{bmatrix} = 0. \tag{17}
\]
By means of \( K_G \), the kernel subspace of \( G \) is defined as
\[
K_G = \left\{ \begin{bmatrix} u \\ y \end{bmatrix} : \begin{bmatrix} -\tilde{N} & \hat{M} \end{bmatrix} \begin{bmatrix} u \\ y \end{bmatrix} = 0, \begin{bmatrix} u \\ y \end{bmatrix} \in \mathcal{L}_2 \right\},
\]
which is, due to relation (16), identical with \( \mathcal{I}_G \), i.e. \( K_G = I_G \) \cite{Vinnicombe2000}. Correspondingly, \( \mathcal{I}_G^\perp \) can be defined by
\[
\mathcal{I}_G^\perp = \left\{ \begin{bmatrix} u \\ y \end{bmatrix} : \begin{bmatrix} -\tilde{N} & \hat{M} \end{bmatrix} \begin{bmatrix} u \\ y \end{bmatrix} \neq 0, \begin{bmatrix} u \\ y \end{bmatrix} \in \mathcal{L}_2 \right\}.
\]
Let \( (\hat{M}_0, \tilde{N}_0) \) be the normalized left coprime pair that, as a dual form of \((M_0,N_0)\), satisfies
\[
\tilde{N}_0(s)\tilde{N}_0^\perp(s) + \hat{M}_0(s)\hat{M}_0^\perp(s) = I. \tag{18}
\]
On account of (15), (16) and (18), we have
\[
\begin{bmatrix} M_0^\perp & N_0^\perp \\ -\tilde{N}_0 & \hat{M}_0 \end{bmatrix} \begin{bmatrix} M_0 & -\tilde{N}_0 \\ N_0 & \hat{M}_0 \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}. \tag{19}
\]
It follows from (19) that
\[
\begin{bmatrix}
u \\ y \end{bmatrix} = \begin{bmatrix} M_0 & -\hat{N}_0^\top \\ \hat{N}_0 & M_0^\top \end{bmatrix} \begin{bmatrix} v \\ q \end{bmatrix} = \begin{bmatrix} M_0 & -\hat{N}_0^\top \\ \hat{N}_0 & M_0^\top \end{bmatrix} q,
\]
\[
\begin{bmatrix} v \\ q \end{bmatrix} = \begin{bmatrix} M_0^\top & -\hat{N}_0^\top \\ -\hat{N}_0 & M_0^\top \end{bmatrix} \begin{bmatrix} u \\ y \end{bmatrix} = \begin{bmatrix} M_0^\top u + \hat{N}_0^\top y \\ \hat{N}_0 y - \hat{N}_0 u \end{bmatrix},
\]
and furthermore
\[
I_G^\perp = \left\{ \begin{bmatrix} u \\ y \end{bmatrix} : \begin{bmatrix} u \\ y \end{bmatrix} = \begin{bmatrix} -\hat{N}_0^\top \\ M_0^\top \end{bmatrix} q, q \in \mathcal{L}_2 \right\}, \tag{20}
\]

**Remark 2** It is noteworthy that the above results on coprime factorizations, orthogonal projections, and image and kernel subspaces hold both for continuous- and discrete-time systems. The reader is referred to Vidyasagar (1985); Hoffmann (1996); Vinnicombe (2000); Ding et al. (2022) for more details about the aforementioned methods.

Now, we delineate how to solve the formulated optimal fault detection problem by means of the system
\[
\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = \Pi \begin{bmatrix} u \\ y \end{bmatrix} = I_{G,0} I_{G,0}^\perp \begin{bmatrix} u \\ y \end{bmatrix},
\]
step by step and on account of the following arguments:

- given process data \((u, y)\) generated by normal operations, there exists \(v \in \mathcal{L}_2\) so that
  \[
  \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = I_{G,0} I_{G,0}^\perp I_{G,0} v = I_{G,0} v \in I_G \implies \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2 = 0;
  \]

- given process data \((u, y)\) generated during operations with disturbances/uncertainties or faults,
  \[
  \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2 = \left\| I_{G,0} I_{G,0}^\perp I_{G,0} v \right\|_2 \neq 0; \tag{21}
  \]

- according to the distance definition (13), the threshold is set to be
  \[
  J_{th} := \sup_{FAR \leq \gamma} \text{dist} \left( \begin{bmatrix} u \\ y \end{bmatrix}, I_G \right)^2 \bigg| 
  \begin{bmatrix} u \\ y \end{bmatrix} \in Z \bigg| \left( u_0 \right) - \left[ \begin{bmatrix} u \\ y \end{bmatrix} \right]_2^2, \tag{22}
  \]
where \(Z\) denotes the set of the process data \((u, y)\) collected during the fault-free operations, and \(\gamma\) is the user-defined FAR upper bound.

The following facts are of remarkable importance in the subsequent study:

- for any \(\begin{bmatrix} u \\ y \end{bmatrix} \in \mathcal{L}_2\),
  \[
  \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = P_{I_G} \begin{bmatrix} u \\ y \end{bmatrix} \in I_G \iff \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = I_{G,0} v, v = I_{G,0}^\perp \begin{bmatrix} u \\ y \end{bmatrix} \in \mathcal{L}_2, \tag{23}
  \]

- moreover,
  \[
  \left\| \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2 = \left\| P_{I_G} \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 = \left\| I_{G,0}^\perp \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 = \left\| v \right\|_2 \tag{24}
  \]

- as well as
  \[
  \left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 = \left\| P_{I_G} \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 \begin{bmatrix} u \\ y \end{bmatrix} \begin{bmatrix} u \\ y \end{bmatrix} = \left\| I_{G,0}^\perp \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 \begin{bmatrix} u \\ y \end{bmatrix} \begin{bmatrix} u \\ y \end{bmatrix} \Rightarrow \left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2^2 = \left\| P_{I_G} \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2^2 + \left\| I_{G,0}^\perp \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2^2 \tag{25}
  \]

As defined in (23), \(v\) is a latent variable for constructing process variables \((u, y)\) in the nominal operation. The fact (24) reveals that \(v\) preserves the exact amount of information needed for constructing the process variables \((u, y)\) in the nominal operation. As the latent variable, \(v\) is achieved by maximally compressed
mapping of \((u, y)\) and preserves as much as possible the information in \((u, y)\) by its reconstruction. Moreover, (21) and (25) imply the maximal sensitivity of the evaluation function to faulty operations. This motivates us to introduce the following definition.

**Definition 1** The property (24) is called lossless information compression.

We would like to mention that the term lossless is a well-established concept in control theory and describes the property of a dynamic system in the regard of energy balance and transport (van der Schaft 2000). For our study on projection-based fault detection, lossless is adopted in the context of information compression and expressed as preservation of the \(L_2\) norm of \(v\) and \((\hat{u}, \hat{y})\). As will be showcased in the next subsection, under certain conditions, the concept of lossless information compressing is equivalent to minimal sufficient statistic for dynamic (control) systems in sense of mutual information.

Guided by the above results, an AE consisting of

\[
\begin{aligned}
\text{encoder: } v &= I_{G, 0} \begin{bmatrix} u \\ y \end{bmatrix}, \\
\text{decoder: } \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} &= I_{G, 0} v,
\end{aligned}
\]

with \(v\) as the latent variable, together with the residual evaluation function \(J\),

\[
J = \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2^2,
\]

as well as the threshold setting law (22) would form an optimal fault detection system that solves the formulated optimal fault detection problem. Unfortunately, the aforementioned results are limited to LTI systems. In the subsequent subsections, we will extend and realize the idea for nonlinear systems and finally propose a learning scheme to train the autoencoder designed based on the idea introduced in this subsection.

### 3.2 Information theoretic view of latent variable learning

In their celebrated review paper on representation learning (Bengio et al. 2013), Bengio et al. have pointed out that by learning the latent variable as feature vector “good generalization means low reconstruction error at test examples, while having high reconstruction error for most other configurations”. In the context of fault detection as a one-class classification problem, this claim implies the maximal fault detectability subject to the required FAR condition. To this aim, the concept of minimal sufficient statistic is helpful (Tishby & Zaslavsky 2015 Geiger 2021). In the information-theoretic framework, learning the latent variable as a minimal sufficient statistic is equivalent to finding a latent representation that minimizes the mutual information of the input and latent variables and simultaneously maximizes the mutual information of the latent and the output variables (Geiger 2021). Concerning our task, this optimization issue is schematically formulated as finding \(v\) so that

\[
I \left( \begin{bmatrix} u \\ y \end{bmatrix} ; v \right) \to \min \quad \text{and} \quad I \left( \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} ; v \right) \to \max.
\]

Here, \(I(X; Y)\) represents the mutual information of two random variables \(X\) and \(Y\), which can be expressed in terms of the entropies of \(X\) and \(Y\), and joint entropy of \(X\) and \(Y\), \(H(X), H(Y), H(X, Y)\), as

\[
I(X; Y) = H(X) + H(Y) - H(X, Y),
\]

and is bounded by \(H(X)\) or \(H(Y)\) (Cover & Thomas 2006). In the sequel, we highlight that the orthogonal projection-based reconstruction with the latent variable \(v\) solves this optimisation problem in a defined probabilistic setting.

To begin with, we briefly review some existing definitions and results in information theory concerning dynamic processes (Papoulis & Pillai 2002 Cover & Thomas 2006). Let \(\{x(k)\}_{k=-\infty}^{\infty}, \{y(k)\}_{k=-\infty}^{\infty}, x \in \mathbb{R}^m, y \in \mathbb{R}^n\), denote discrete-time stationary stochastic processes. The entropy rate of \(\{x(k)\}_{k=-\infty}^{\infty}\), and the mutual information rate of \(\{x(k)\}_{k=-\infty}^{\infty}, \{y(k)\}_{k=-\infty}^{\infty}\) represent the limits of the average entropy and average mutual information, respectively, and are defined by

\[
H_R(x) := \lim_{n \to \infty} \frac{1}{n} H(x(1), \cdots, x(n)),
\]

\[
I_R(x; y) := \lim_{n \to \infty} \frac{1}{n} I(x(1), \cdots, x(n); y(1), \cdots, y(n)).
\]

Denote by \(\Phi_x(\theta), \Phi_y(\theta)\) and \(\Phi_{xy}(\theta)\), \(\Phi_{yx}(\theta), \theta \in [-\pi, \pi]\), the power spectral densities and cross-power spectral densities of \(x\) and \(y\), respectively. Note that

\[
\Phi_{xy}(\theta) = \Phi_{yx}^*(-\theta) = \Phi_{yx}(\theta).
\]

**Remark 3** Power and cross-power spectral densities \(\Phi_x(\theta)/\Phi_y(\theta)\) and \(\Phi_{xy}(\theta)\) are the discrete-time Fourier transform of the corresponding autocorrelation and cross-correlation functions. Variable \(\theta\) denotes the frequency (Boashash 2015).

We are in the position to introduce the major result in this subsection. The following lemmas are essential for our work.
Lemma 1 (Cover & Thomas, 2006; Ishii et al., 2011) Given a zero-mean asymptotically stationary Gaussian process \( \{ x(k) \}_{k=-\infty}^{\infty}, x \in \mathbb{R}^n \), with power spectral density \( \Phi_x(\theta) \), then

\[
H_R(x) = \frac{1}{2} \log (2\pi e)^n + \frac{1}{4\pi} \int_{-\pi}^{\pi} \log \det \Phi_x(\theta) d\theta. \tag{26}
\]

Lemma 2 (Pinsker, 1964; Stoorvogel & van Schuppen, 1996; Zhang & Sun, 2005) Given two zero-mean asymptotically stationary Gaussian processes \( \{ x(k) \}_{k=-\infty}^{\infty}, \{ y(k) \}_{k=-\infty}^{\infty}, x \in \mathbb{R}^n, y \in \mathbb{R}^m \), and the joint Gaussian process \( \zeta(k) = \begin{bmatrix} x(k) \\ y(k) \end{bmatrix} \in \mathbb{R}^{n+m} \) with power spectral densities \( \Phi_x(\theta), \Phi_y(\theta) \) as well as \( \Phi_\zeta(\theta) \), then mutual information rate of \( x \) and \( y \) is given by

\[
I_R(x;y) = \frac{1}{4\pi} \int_{-\pi}^{\pi} \log \frac{\det \Phi_\zeta(\theta) \det \Phi_y(\theta)}{\det \Phi_\zeta(\theta)} d\theta. \tag{27}
\]

In order to fit the above information theoretic setting, we now consider, analog to continuous-time systems, discrete-time system models and the associated RCF and LCF as well as the normalized SIR and SKR,

\[
I_{G,0}(z) = \begin{bmatrix} M_0(z) \\ N_0(z) \end{bmatrix}, \quad K_{G,0}(z) = \begin{bmatrix} \tilde{N}_0(z) & M_0(z) \end{bmatrix},
\]

the orthogonal projection \( \mathcal{P}_{I_G} \), as described in the previous subsection. The problem under consideration is formulated as follows: given system

\[
\begin{bmatrix} u \\ y \end{bmatrix} = I_{G,0} \bar{v} + K_{G,0} q, \quad v = I_{G,0} \begin{bmatrix} u \\ y \end{bmatrix} + \xi, \tag{28}
\]

\[
\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = I_{G,0} v, \quad K_{G,0}^\sim = \begin{bmatrix} \tilde{N}_0^\sim \\ \tilde{M}_0^\sim \end{bmatrix}, \tag{29}
\]

where \( \bar{v} \in \mathcal{L}_2 \) is a deterministic signal and represents nominal operations, \( q, \xi \) are zero-mean stationary Gaussian processes, and \( K_{G,0}^\sim q \) and \( \xi \) are independent, find \( I_R \left( \begin{bmatrix} u \\ y \end{bmatrix} ; v \right) \) and \( I_R \left( \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} ; v \right) \). Recall that \( K_{G,0}^\sim q \in I_G^\sim \) represents uncertainties caused by disturbances or/and faulty operations. Thus, the mutual information rate

\[
I_R \left( \begin{bmatrix} u \\ y \end{bmatrix} ; v \right)\]

indicates amount of uncertainties in the latent variable \( v \).

Theorem 1 Given system (28)-(29) with the asymptotically stationary Gaussian processes \( \begin{bmatrix} u \\ y \end{bmatrix}, \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \) and \( v \), it holds

\[
I_R \left( \begin{bmatrix} u \\ y \end{bmatrix} ; v \right) = 0, H_R(v) = H_R \left( \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right). \tag{30}
\]

Proof. Let

\[
\beta = \begin{bmatrix} u \\ y \end{bmatrix} - \mathbb{E} \left( \begin{bmatrix} u \\ y \end{bmatrix} \right) = \begin{bmatrix} u \\ y \end{bmatrix} - I_{G,0} \bar{v} = K_{G,0}^\sim q, \alpha = v - \mathbb{E}(v) = I_{G,0} K_{G,0}^\sim q + \xi,
\]

where \( \mathbb{E}(\cdot) \) denotes expectation. Hence, both \( \alpha \) and \( \beta \) are zero-mean asymptotically stationary Gaussian processes. It follows from Lemma 2 that

\[
I_R \left( \begin{bmatrix} u \\ y \end{bmatrix} ; v \right) = \frac{1}{4\pi} \int_{-\pi}^{\pi} \log \frac{\det \Phi_\beta(\theta) \det \Phi_\alpha(\theta)}{\det \Phi_\gamma(\theta)} d\theta, \tag{31}
\]

\[
\gamma = \begin{bmatrix} \beta \\ \alpha \end{bmatrix}, \Phi_\gamma(\theta) = \begin{bmatrix} \Phi_\beta(\theta) & \Phi_{\beta\alpha}(\theta) \\ \Phi_{\alpha\beta}(\theta) & \Phi_\alpha(\theta) \end{bmatrix}, \tag{32}
\]

\[
\Phi_{\beta\alpha}(\theta) = \Phi_\beta(\theta) I_{G,0}(\theta). \tag{33}
\]

Since

\[
\Phi_\beta(\theta) = K_{G,0}^\sim(\theta) \Phi_q(\theta) K_{G,0}(\theta), K_{G,0}(\theta) I_{G,0}(\theta) = 0, \quad \text{and} \quad K_{G,0}^\sim q \text{ and } \xi \text{ are independent, it turns out}
\]

\[
\log \frac{\det \Phi_\beta(\theta) \det \Phi_\alpha(\theta)}{\det \Phi_\gamma(\theta)} = 0 \implies I_R \left( \begin{bmatrix} u \\ y \end{bmatrix} ; v \right) = 0.
\]

Recall (19), namely

\[
\begin{bmatrix} I_{G,0}^\sim \\ K_{G,0} \end{bmatrix} \begin{bmatrix} I_{G,0}^\sim \\ K_{G,0} \end{bmatrix}^\sim = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix},
\]

which means that \( I_{G,0}^\sim \) is a unitary mapping.
Multiplying $\begin{bmatrix} \dot{u} \\ \dot{y} \end{bmatrix}$ by $\begin{bmatrix} I_{G,0} \\ K_{G,0} \end{bmatrix}$ yields
\[
\begin{bmatrix} I_{G,0} \\ K_{G,0} \end{bmatrix} \begin{bmatrix} \dot{u} \\ \dot{y} \end{bmatrix} = I_{G,0}v = \begin{bmatrix} v \\ 0 \end{bmatrix}.
\]
As a result, by Lemma 1
\[
H_R \left( \begin{bmatrix} \dot{u} \\ \dot{y} \end{bmatrix} \right) = H_R (v) \quad (34)
\]
\[
= \frac{1}{2} \log (2\pi e)^p + \frac{1}{4\pi} \int_{-\pi}^{\pi} \log \det \Phi_u(\theta) d\theta.
\]
The theorem is thus proven. ■

Note that the relation (34) implies that $I_R \left( \begin{bmatrix} \dot{u} \\ \dot{y} \end{bmatrix} : v \right)$ is equal to its upper-bound and thus reaches the maximum. In summary, Theorem 1 gives a solution to the optimal selection of the latent variable and proves that the latent variable $v = I_{G,0} \begin{bmatrix} u \\ y \end{bmatrix}$ is a minimal sufficient statistic on the assumption of the system model (28)-(29). In particular, the relation (30) provides us with an information theoretic interpretation for the concept of lossless information compression given in Definition 1. We would like to emphasize that the property (30) is the result of the adopted orthogonal projection and leads to the maximal fault detectability thanks to the maximal sensitivity of the evaluation function to the faulty operations.

### 3.3 Extension to nonlinear dynamic systems

We now consider nonlinear systems given in (1). For the sake of simplicity, we restrict our study to a class of nonlinear systems, the so-called affine systems modelled by the following state space representation
\[
\Sigma : \begin{cases} \dot{x} = a(x) + B(x)u \\ y = c(x) + D(x)u, \end{cases} \quad (35)
\]
where $a(x), B(x), c(x), D(x)$ are smooth functions of appropriate dimensions. Analog to LTI systems, the definition of stable image representation of $\Sigma$ is essential for our extension effort.

**Definition 2** (van der Schaft [2000]) Given system $\Sigma$ defined by (35), system $\Sigma_I : \mathcal{V} \rightarrow \mathcal{L}_2 \times \mathcal{L}_2$ is an SIR of the system $\Sigma$ if for all $u \in \mathcal{U} \subseteq \mathcal{L}_2$ and $y = \Sigma(u) \in \mathcal{Y} \subseteq \mathcal{L}_2$, there exists $v \in \mathcal{V} \subseteq \mathcal{L}_2$ such that
\[
\begin{bmatrix} u \\ y \end{bmatrix} = \Sigma_I (v).
\]

A state space representation of the SIR is given by
\[
\Sigma_I : \begin{cases} \dot{x} = a(x) + B(x)g(x) + B(x)V(x)v \\ y = \bar{u}(x) + B(x)V(x)v \end{cases}, \quad (36)
\]
\[
\bar{c}(x) = \begin{bmatrix} g(x) \\ c(x) + D(x)g(x) \end{bmatrix}, \quad \bar{D}(x) = \begin{bmatrix} V(x) \\ D(x)V(x) \end{bmatrix},
\]
where $g(x)$ is designed such that $\bar{u}(x) = a(x) + B(x)g(x)$ is asymptotically stable and $V(x) \in \mathbb{R}^{p \times p}$ is invertible [Scherpen & van der Schaft 1994; Ball & van der Schaft 1996]. In the context of feedback control systems,
\[
u = g(x) + V(x)v
\]
can be understood as a controller with state feedback $g(x)$, feed-forward controller $V(x)$ and $v$ as the reference signal. Note that
\[
\bar{D}^T(x)\bar{D}(x) = V^T(x) (I + D^T(x)D(x)) V(x)
\]
is invertible.

Based on the SIR of $\Sigma$, the image subspace of $\Sigma$, which defines the set of the process data generated under the nominal operation conditions, is defined as follows.

**Definition 3** Given system $\Sigma$, its SIR $\Sigma_I$, and $u \in \mathcal{U}, y \in \mathcal{Y}$,
\[
\mathcal{I}_\Sigma = \left\{ \begin{bmatrix} u \\ y \end{bmatrix} : \begin{bmatrix} u \\ y \end{bmatrix} = \Sigma_I (v), v \in \mathcal{V} \right\} \quad (37)
\]
is called image subspace of $\Sigma$.

Recall that for LTI systems, the basic idea of constructing an optimal fault detection system is to find an operator $\Pi$,
\[
\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = \Pi \begin{bmatrix} u \\ y \end{bmatrix},
\]
which is idempotent, i.e.
\[
\Pi \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = \Pi \left( \Pi \begin{bmatrix} u \\ y \end{bmatrix} \right) = \Pi \begin{bmatrix} u \\ y \end{bmatrix}, \quad (38)
\]
and guarantees lossless information compression, as defined in Definition 1,

\[ \|v\|_2 = \left\| \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2 = \left\| \Pi \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2. \quad (39) \]

For LTI systems, the normalized SIR serves for this end with \( \Pi = I_{G,0}I_{G,0}^\top \), which cannot be applied to nonlinear systems. Notice that the conditions (38)-(39) are essential for the orthogonal projection. It inspires us to address the issues for nonlinear systems under these two aspects. To this end, the concepts of the Hamiltonian extension and inner systems are firstly introduced, which are well established in nonlinear control theory \cite{Crouch1987, Scherpen1994}.

Given system (36), the Hamiltonian extension of \( \Sigma_I \) is a dynamic system described by

\[
\begin{aligned}
\dot{x} &= \hat{a}(x) + B(x)v \\
\dot{p} &= -\left( \frac{\partial \hat{a}(x)}{\partial x} + \frac{\partial B(x)}{\partial x} \right) v_a, \\
\vec{z} &= \begin{bmatrix} u \\ y \end{bmatrix} = \vec{c}(x) + \vec{D}(x)v \\
z_a &= B^T(x)p + \vec{D}^T(x)v_a, z_a \in \mathbb{R}^p, v_a \in \mathbb{R}^{m+p}
\end{aligned}
\]

with state variables \((x, p)\), \(p \in \mathbb{R}^a\), input variables \((v, v_a)\) and output variable \((\vec{z}, z_a)\). Define the Hamiltonian function

\[
H(x, p, v) = \frac{1}{2} \left( \vec{c}(x) + \vec{D}(x)v \right)^T \left( \vec{c}(x) + \vec{D}(x)v \right) + p^T \left( \hat{a}(x) + B(x)v \right)
\]

and connect \(\vec{z}\) and \(v_a, v_a = \vec{z} = \vec{c}(x) + \vec{D}(x)v\). We have the following Hamiltonian system

\[
z_a = (D\Sigma_I)^T \circ \Sigma_I (v),
\]

whose state space representation can be written in the compact form

\[
(D\Sigma_I)^T \circ \Sigma_I : \begin{cases} 
\dot{x} = \frac{\partial H}{\partial x}(x, p, v) \\
\dot{p} = -\frac{\partial H}{\partial p}(x, p, v), \\
z_a = \frac{\partial H}{\partial v_a}(x, p, v).
\end{cases} \quad (41)
\]

We now introduce the definition of inner systems \cite{Scherpen1994}.

**Definition 4** Given nonlinear affine system (36) and the corresponding Hamiltonian system (41), \( \Sigma_I \) is inner if

\[
z_a = v, \quad (42)
\]

and there exists a storage function \( P(x) \geq 0, P(0) = 0 \) so that

\[
P(x(t_2)) - P(x(t_1)) = \int_{t_1}^{t_2} \left( \frac{1}{2} v^T v - \frac{1}{2} \vec{z}^T \vec{z} \right) \, dt. \quad (43)
\]

**Remark 4** A system with the property (43) is called lossless with respect to the supply rate

\[
s(v, \vec{z}) = \frac{1}{2} v^T v - \frac{1}{2} \vec{z}^T \vec{z}.
\]

For \( t_1 = 0, t_2 = \infty, x(0) = 0 \), it holds

\[
\int_0^\infty \left( \frac{1}{2} v^T v - \frac{1}{2} \vec{z}^T \vec{z} \right) \, dt = 0
\]

\[
\iff \|v\|_2 = \|\vec{z}\|_2 = \left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2.
\]

The existence conditions for the system (36) to be inner are summarized in the following lemma.

**Lemma 3** The nonlinear affine system (36) is inner, if there exists \( P(x) \geq 0 \) such that the following equations are feasible

\[
\begin{aligned}
P_x(x) \hat{a}(x) + \frac{1}{2} \hat{c}(x)\hat{c}(x) &= 0, \\
P_x(x) B(x) + \frac{1}{2} \hat{c}(x)\hat{D}(x) &= 0, \\
\hat{D}(x)\hat{D}(x) &= I,
\end{aligned}
\]

where \( P_x(x) = \frac{\partial P}{\partial x}(x) \).

The results given in the above lemma are well-known, see, for instance, Scherpen & van der Schaft (1994); Ball & van der Schaft (1996). Hence, the proof of Lemma 3 is omitted.

According to Lemma 3, the SIR \( \Sigma_I \) becomes inner, when feedback and feed-forward controllers \( g(x) \) and \( V(x) \) are set in such a way such that equations (44)-(46) are solved.

Let \( \Sigma_I \) be inner, and denoted by \( \Sigma_{I,0} \). We propose to build estimator \( \Pi \) as follows

\[
\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = \Pi \begin{bmatrix} u \\ y \end{bmatrix} = \Sigma_{I,0} \circ (D\Sigma_{I,0})^T \begin{bmatrix} u \\ y \end{bmatrix}, \quad (47)
\]

whose state space representation is, by connecting \( z_a \) and \( v \) in the Hamiltonian extension (40) and defining

\[
v_a = \begin{bmatrix} u \\ y \end{bmatrix},
\]

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Moreover, due to the lossless property of $\Sigma_{I,0}$, given by

$$
\Sigma_{I,0} \circ (D\Sigma_{I,0})^T : \begin{cases}
\dot{x} = \bar{a}(x) + B(x)B^T(x)p + B(x)\bar{D}^T(x) \begin{bmatrix} u \\ y \end{bmatrix} \\
\dot{p} = -\left(\frac{\partial \bar{a}(x)}{\partial x} + \frac{\partial}{\partial x} B(x) \left( B^T(x)p + \bar{D}^T(x) \begin{bmatrix} u \\ y \end{bmatrix} \right) \right)^T \begin{bmatrix} u \\ y \end{bmatrix} \\
\begin{bmatrix} \dot{\hat{u}} \\ \dot{\hat{y}} \end{bmatrix} = \bar{c}(x) + \bar{D}(x)B^T(x)p + \bar{D}(x)\bar{D}^T(x) \begin{bmatrix} u \\ y \end{bmatrix}.
\end{cases}
$$

which results in

$$
\left\| (D\Sigma_{I,0})^T \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 = \|v\|_2 = \|\Sigma_{I,0}(v)\|_2
$$

Theorem 2: Given system (47), it holds

$$
\Sigma_{I,0} \circ (D\Sigma_{I,0})^T \circ \Sigma_{I,0} \circ (D\Sigma_{I,0})^T \begin{bmatrix} u \\ y \end{bmatrix} = \Sigma_{I,0} \circ (D\Sigma_{I,0})^T \begin{bmatrix} u \\ y \end{bmatrix},
$$

and

$$
\left\| (D\Sigma_{I,0})^T \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 = \|v\|_2 = \|\Sigma_{I,0}(v)\|_2
$$

The theorem is thus proven. ■

In the context of fault detection, Theorem 2 implies that

- $\forall \begin{bmatrix} u \\ y \end{bmatrix} \in \mathcal{I}_\Sigma$, i.e. process data generated under the nominal operation condition,

$$
\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = \Pi \begin{bmatrix} u \\ y \end{bmatrix} = \Sigma_{I,0}(v) = \begin{bmatrix} u \\ y \end{bmatrix},
$$

- the generation of the latent variable by

$$
\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = \Sigma_{I,0}(v)
$$

is a lossless information compression, and

- $\forall \begin{bmatrix} u \\ y \end{bmatrix} \notin \mathcal{I}_\Sigma$,

$$
\left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 \geq \left\| \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2 = \|v\|_2,
$$

$$
\implies \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2 \geq 0.
$$

As a result, the formulated optimal fault detection problem can be solved by (i) constructing an AE realizing

$$
\begin{align*}
\text{encoder: } v &= (D\Sigma_{I,0})^T \begin{bmatrix} u \\ y \end{bmatrix}
\end{align*}
$$

(49)

with $\hat{v}$ as the latent variable, (ii) defining the evaluation
function

\[ J = \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2^2 = \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \Sigma_{I,0}(v) \right\|_2^2, \]  

and setting the threshold as

\[ J_{th} = \sup_{u,y \in Z, \text{FAR} \leq \gamma} \text{dist} \left( \begin{bmatrix} u \\ y \end{bmatrix}, \Sigma_{I} \right)^2, \]

\[ Z = \mathcal{U} \times \mathcal{Y}, \text{FAR} \leq \gamma \]

\[ = \sup_{u,y \in Z, u_0 \in \Sigma_{I}, y_0 \in \mathcal{Y}} \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} u_0 \\ y_0 \end{bmatrix} \right\|_2^2. \]  

(51)

It is obvious that the above solution can only be analytically achieved if (i) the process model (35) exists, and (ii) \( g(x) \) and \( V(x) \) in the SIR \( \Sigma_{I,0} \) can be determined by solving equations (44)-(46). In practical applications, both of these requirements can often not be satisfied or are satisfied at remarkably high engineering costs. In the next subsection, we are going to introduce a data-driven solution alternatively using an AE that will be learnt in such a way that it is idempotent and results in lossless information compression via the latent variable \( v \).

3.4 An AE-based fault detection scheme

We now propose a learning algorithm to train an AE to realize the optimal fault detection system given in (49)-(51) on the assumption that

- sufficient process data \((u, y)\) have been collected during fault-free operations,
- the data have been recorded batchwise,
- \( u^{(i)} \)
- \( y^{(i)} \)

\[ \begin{bmatrix} u^{(i)} \\ y^{(i)} \end{bmatrix} = \begin{bmatrix} u^{(k)} \\ y^{(k)} \end{bmatrix}, k \in [k_i, k_i + N], \]

where \( k, k_i \) are the sampling number, \( N \) is the length of the data batch, and
- the data set is denoted by \( Z \),

\[ Z = \left\{ \begin{bmatrix} u^{(i)} \\ y^{(i)} \end{bmatrix}, i = 1, \cdots M \right\}. \]

For our purpose,

- recurrent neural networks (RNNs) are firstly constructed as

\[ \begin{aligned}
\text{encoder:} \quad & \mathcal{RNN}_{en}(\theta_{en}, \begin{bmatrix} u \\ y \end{bmatrix}) = (D \Sigma_{I,0})^T \begin{bmatrix} u \\ y \end{bmatrix} = v \\
\text{decoder:} \quad & \mathcal{RNN}_{de} (\theta_{de}, v) = \Sigma_{I,0}(v) = \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix},
\end{aligned} \]  

(52)

and they build an AE, based on it,
- the evaluation function is computed (during training and later for the online implementation)

\[ J = \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2^2 = \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \mathcal{RNN}_{de}(\theta_{de}, v) \right\|_2^2 
\]

\[ = \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \mathcal{RNN}_{de}(\theta_{de}, \mathcal{RNN}_{en}(\theta_{en}, \begin{bmatrix} u \\ y \end{bmatrix})) \right\|_2^2, \]

after the AE is learnt, and finally
- the threshold is to be determined as

\[ J_{th} = \sup_{\begin{bmatrix} u^{(i)} \\ y^{(i)} \end{bmatrix} \in Z, \text{FAR} \leq \gamma} \left\| \begin{bmatrix} u^{(i)} \\ y^{(i)} \end{bmatrix} - \hat{u}^{(i)} \right\|_2^2. \]

\[ \hat{u}^{(i)} = \mathcal{RNN}_{de}(\theta_{de}, \mathcal{RNN}_{en}(\theta_{en}, \begin{bmatrix} u^{(i)} \\ y^{(i)} \end{bmatrix})). \]

We would like to remark that process data \((u, y)\) exist generally as discrete-time samples. Correspondingly, the \( L_2 \) norm adopted in the evaluation function is approximated by

\[ ||a||^2_2 := \sum_{i=k_0}^{k_0+N} a^T(i) a(i). \]

Next, as a major contribution of our work, the loss function for optimizing the parameters \( \theta_{en}, \theta_{de} \) of RNNs is defined. In order to learn an idempotent autoencoder with lossless information compression, two regularized terms, \( \mathcal{L}_2(\theta_{de}, \theta_{en}) \) and \( \mathcal{L}_3(\theta_{de}, \theta_{en}) \), are introduced into the loss function, in addition to the standard index,

\[ \mathcal{L}_1(\theta_{de}, \theta_{en}) = \frac{1}{M} \sum_{i=1}^{M} \left\| \begin{bmatrix} u^{(i)} \\ y^{(i)} \end{bmatrix} - \hat{u}^{(i)} \right\|_2^2. \]  

(53)

It is obvious that \( \mathcal{L}_1(\theta_{de}, \theta_{en}) \) is dedicated to minimizing
the reconstruction error and thus the evaluation function

\[ J = \left\| \begin{bmatrix} u \\ y \end{bmatrix} - \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \right\|_2^2. \]

The two regularized terms are

\[
\mathcal{L}_2(\theta_{de}, \theta_{en}) = \frac{1}{M} \sum_{i=1}^{M} \left\| \begin{bmatrix} \tilde{u}(i) \\ \tilde{y}(i) \end{bmatrix} - \mathcal{RNN}_{de}(\theta_{de}, \mathcal{RNN}_{en}(\theta_{en}, \begin{bmatrix} \tilde{u}(i) \\ \tilde{y}(i) \end{bmatrix})) \right\|_2^2,
\]

\[
\mathcal{L}_3(\theta_{de}, \theta_{en}) = \frac{1}{M} \sum_{i=1}^{M} \left\| \mathcal{RNN}_{en}(\theta_{en}, \begin{bmatrix} u(i) \\ y(i) \end{bmatrix}) - \mathcal{RNN}_{en}(\theta_{en}, \begin{bmatrix} \hat{u}(i) \\ \hat{y}(i) \end{bmatrix}) \right\|_2^2,
\]

which implies that the AE is inner. Consequently,

\[
\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} = \langle v, \mathcal{RNN}_{en}(\theta_{en}, \mathcal{RNN}_{de}(\theta_{de}, v)) \rangle,
\]

\[
\begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} - \| v \|_2 \to 0,
\]

which results in lossless information compression. Finally, we have the total loss function \( \mathcal{L}(\theta_{en}, \theta_{de}) \) given by

\[
\mathcal{L}(\theta_{en}, \theta_{de}) = \sum_{i=1}^{3} \omega_i \mathcal{L}_i(\theta_{en}, \theta_{de}),
\]

where \( 0 < \omega_i \leq 1 \) denotes a weighting factor. Fig. 3 sketches the learning procedure proposed above, in which

- the NNs, \( \mathcal{RNN}_{en}(\theta_{en}, \begin{bmatrix} u(i) \\ y(i) \end{bmatrix}) \), \( \mathcal{RNN}_{de}(\theta_{de}, v) \), in the AE block are learnt using an optimization algorithm,
- \( \begin{bmatrix} \hat{u} \\ \hat{y} \end{bmatrix} \) and \( \hat{v} \) are the intermediate variables used for the calculation of the regularized terms \( \mathcal{L}_2(\theta_{de}, \theta_{en}) \) and \( \mathcal{L}_3(\theta_{de}, \theta_{en}) \), which, together with the latent variable \( v \), process data \( \begin{bmatrix} u \\ y \end{bmatrix} \) and \( \mathcal{L}_1(\theta_{en}, \theta_{de}) \), build the loss function \( \mathcal{L}(\theta_{en}, \theta_{de}) \) for the optimization.

We name the above AE Inner-Autoencoder (I-AE). It is worth to emphasize that the I-AE-based solution proposed above is a pure data-driven solution. It requires (i) no process model, e.g. as given by (35), and (ii) no solution of differential equations like (44)-(46). So far, it is a general and practical solution for detecting faults in nonlinear dynamic systems.

### 4 Data experimental study

In this section, the main results of our work on control theoretically guided training of autoencoders for detecting faults in nonlinear dynamic processes are evaluated on a three-tank system simulator. The objective of the evaluation study is twofold:

- comparison of the I-AE trained under the loss function (56) with a standard AE regarding their capability of performing fault detection,
• explanation of the role of the latent variable in approaching an optimal fault detection.

4.1 Experimental setting and data description

Three-tank systems (TTS) have typical characteristics of chemical processes and are widely accepted as a benchmark process in research and application domains of process control and fault diagnosis. The simulator adopted in our work is the real-time laboratory setup TTS20 that is in operation in the AKS labor since more than 20 years (Ding, 2008, 2020). As schematically sketched in Fig. 4, TTS20 consists of three water tanks that are connected through pipes. Water from a reservoir is pumped into tank 1 and tank 2, respectively. TTS20 is a nonlinear dynamic control system. Two input variables, \( u_1 \) and \( u_2 \), manipulate the incoming mass flow into tank 1 and tank 2. In order to regulate the water levels in tank 1 and tank 2, two PI-controllers are used with the output variables \( y_1 \) and \( y_2 \), which are measured by two level sensors. The reader is referred to Ding (2014, 2020) for a detailed description of the nonlinear dynamic model, the asset and controller parameters. The simulator has been developed in the MATLAB/SIMULINK software environment with a sampling time equal to 1 s, and simulated sensor and actuator noises. It demonstrates excellent simulation results, and is widely used in teaching programs and research projects.

4.2 Design of evaluation program and data description

In order to guarantee that the NNs to be learnt fully model the nonlinear system dynamics, the reference signals are randomly generated so that over 85% of the operation region of the process are covered. An example is given in Fig. 5, which shows the water level in tank 1, \( y_1 \), with reference signal \( y_{1\text{ref}} \).

To prepare the training data, 1,200,000 fault-free samples are continuously generated by TTS20-simulator. They are randomly divided into a training set and a validation set in a ratio of 7:3. The following three types of faults are simulated:

• 10% leakage fault in tank 1,
• 5% sensor gain fault in the water level sensor mounted on tank 2,
• sensor gain fault in the water level sensor mounted on tank 2 with stepwise changes from 5% to 10% and 15%.

To achieve a reliable fault detection, a moving window with the window length equal to 100 s is adopted for the evaluation purpose.

4.3 Configuration of autoencoders and training

Recurrent neural networks (RNNs) are known to be capable of learning time evolutionary features of dynamic systems. For our purpose, a typical RNN, the long short-term memory (LSTM) NN (Hochreiter & Schmidhuber, 1997), is applied for building the autoencoder. In our experiments, the following hyperparameter combination is adopted:

• four layers in the encoder and decoder, respectively,
• two LSTM units are included in each layer.

With these hyperparameters, all models presented below are set and trained.

In order to showcase the capability of the control theoretically guided autoencoder learning, two autoencoders are trained by means of two different loss functions. The autoencoder trained under the loss function \( \mathcal{L}(\theta_{de}, \theta_{en}) \),

\[
\mathcal{L}(\theta_{de}, \theta_{en}) = \mathcal{L}_1(\theta_{de}, \theta_{en}) = \frac{1}{M} \sum_{i=1}^{M} \left\| \begin{bmatrix} u^{(i)} \\ y^{(i)} \end{bmatrix} - \begin{bmatrix} \hat{u}^{(i)} \\ \hat{y}^{(i)} \end{bmatrix} \right\|^2,
\]

is denoted by AE with \( \mathcal{L}_1 \), while the I-AE trained by the loss function \( \mathcal{L}(\theta_{de}, \theta_{en}) \) given in (56), i.e.

\[
\mathcal{L}(\theta_{en}, \theta_{de}) = \sum_{i=1}^{3} \mathcal{L}_i(\theta_{en}, \theta_{de}).
\]
In Fig. 6, the values of the loss functions of both AEs during the training process are shown for comparison. It is apparent that

- in both cases, the training process converges properly, and
- the AE with $\mathcal{L}_1$ is learnt faster with a smaller reconstruction error than I-AE.

Moreover, according to the final reconstruction error and on the demand for an FAR upper bound equal to 0.05, threshold is set to be 0.2201.

4.4 Fault detection performance evaluation

The trained AE-based fault detection systems, AE with $\mathcal{L}_1$ and I-AE, are tested aiming at examining and comparing their fault detection performance. To this end, the following tests are designed:

- the TTS20-simulator runs for 400s under fault-free operation conditions, and a fault is injected at the time instant 401s with a duration of 400s,
- the AE-based fault detection system runs for 800s, and
- the above procedure is repeated 1000 times under random operation conditions.

Fig. 7 and Fig. 8 are examples of fault detection results. Although these examples show a better detection performance of I-AE than the one of the conventional AE with $\mathcal{L}_1$, performance evaluation metric statistics based on the simulation data are necessary for a reasonable and comparable performance assessment. To this end, FAR and missed detection rate (MDR) as well as accuracy and F1-score that are commonly adopted for anomaly detection (Fawcett, 2006) are under consideration. They are estimated using the detection data as follows:

$$\text{FAR} = \frac{N_{\text{FA}}}{N_{\text{FF}}}, \quad \text{MDR} = \frac{N_{\text{MD}}}{N_{\text{F}}},$$

$$\text{Accuracy} = \frac{N - N_{\text{FA}} - N_{\text{MD}}}{N}, \quad N = N_{\text{F}} + N_{\text{FF}},$$

$$\text{F1-score} = \frac{N_{\text{F}} - N_{\text{MD}}}{N_{\text{F}} - N_{\text{MD}} + \frac{1}{2}(N_{\text{FA}} + N_{\text{MD}})}.$$ 

where $N_{\text{F}}$ and $N_{\text{FF}}$ are the total numbers of faulty and fault-free operations, and $N_{\text{FA}}$ and $N_{\text{MD}}$ are the numbers of false alarms and miss detections, respectively. Thus, $N - N_{\text{FA}} - N_{\text{MD}}$ is the total number of correct decisions, $N_{\text{F}} - N_{\text{MD}}$ is the number of correctly detected faults, and $N$ is the total number of the operations.
Table 1
Fault detection performance evaluation

|                      | AE with $\mathcal{L}_1$ | I-AE     |
|----------------------|--------------------------|----------|
| FAR                  | 0.051±0.004              | 0.049±0.007 |
| MDR                  | 0.441±0.039              | 0.034±0.002 |
| Accuracy             | 0.537±0.038              | 0.915±0.011 |
| F1-score             | 0.267±0.106              | 0.916±0.013 |

Remark 5 Let faulty and fault-free operations be positive and negative classes, respectively. In the framework of anomaly detection [Fawcett 2006], $N_F$ and $N_{FF}$ correspond to the total numbers of positive class and negative class, and $N_{FA}$ and $N_{MD}$ are the numbers of false positives and false negatives, respectively.

In Table 1, the performance evaluation results are listed for both AEs. It is obvious that

- both AEs are at the similar FAR level about 0.05, as required,
- the I-AE is of a considerably lower MDR than the conventional AE with $\mathcal{L}_1$, and consequently,
- accuracy and F1-score of the I-AE are remarkably higher than the ones of the conventional AE with $\mathcal{L}_1$.

4.5 Test on the role of latent variable

To illustrate the influence of the proposed regularized terms on the latent variable in the I-AE and hence to gain a deeper insight into the role of the latent variable, an ablation study is designed as follows: a third AE, named AE with $\mathcal{L}_1 \sim \mathcal{L}_4$, is trained under the loss function

$$\mathcal{L}(\theta_{en}, \theta_{de}) = \sum_{i=1}^{3} \mathcal{L}_i + 0.001 \mathcal{L}_4,$$

where $\mathcal{L}_i$, $i = 1, 2, 3$, are the ones given in (53)-(55), and $\mathcal{L}_4$ is an additional regularized term defined by

$$\mathcal{L}_4(\theta_{en}) = \left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 \left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 - \left\| \mathcal{N} \mathcal{N}_{en} \left( \theta_{en}, \begin{bmatrix} u \\ y \end{bmatrix} \right) \right\|_2 \left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 \right\|_2$$

that minimizes $\left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 \left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2 - \left\| \mathcal{N} \mathcal{N}_{en} \left( \theta_{en}, \begin{bmatrix} u \\ y \end{bmatrix} \right) \right\|_2 \left\| \begin{bmatrix} u \\ y \end{bmatrix} \right\|_2$ . With $\mathcal{L}_4$, the latent variable $v$ will tend to preserve all the information in $u$ and $y$, including uncertainty and redundancy. In other words, $v$ contains, under such a training condition, the information about more than the nominal operations. In the information theoretical context, the latent variable $v$ is no more minimal sufficient statistic. Due to the large amplitude of $\mathcal{L}_4$, it is weighted by a factor 0.001. The training loss of AE with $\mathcal{L}_1 \sim \mathcal{L}_4$ is shown in Fig. 9.

The loss values of AE with $\mathcal{L}_1 \sim \mathcal{L}_4$ are small but not stable enough to fully converge, indicating that there is a contradiction between $\mathcal{L}_4$ and the other loss terms. To assess the fault detection performance and to compare with the other two AEs, the same tests on detecting the sensor gain fault in the water level sensor mounted
on tank 2 with stepwise changes from 5% to 10% and 15% are conducted. A test example is shown in Fig. 10, while the detection performance evaluation results are summarized in Table 2. It can be clearly seen that the introduction of $\mathcal{L}_4$ in the loss function results in an AE-based detection system with degraded fault detectability in comparison with I-AE, the AE trained with a loss function consisting of the regularized terms $\mathcal{L}_2$ and $\mathcal{L}_3$. This result impressively demonstrates the role of a latent variable as a minimal sufficient statistic.

### 4.6 Analysis and summary

As a summary of the experimental results, the following conclusions can be drawn:

- Although the training process of the standard AE shows a higher convergence rate and lower loss function value in comparison with the training process of the I-AE, the I-AE demonstrates a remarkably higher fault detectability, while the requirement on FAR is satisfied.

- These experimental results verify our theoretical results: the fault detection system, consisting of (49) as the estimator (residual generator), (50) as the residual evaluator and (51) as the threshold, delivers the solution to the optimal fault detection problem for nonlinear dynamic systems, formulated as maximizing fault detectability while satisfying the FAR requirement. In this context, the control theoretic results serve as a meaningful guideline for training the I-AE.

- The reason behind these impressive results is that the I-AE is an inner system, which ensures lossless information compression via the latent variable, and consequently leads to maximal fault detectability, and this is achieved by means of introducing the regularized terms $\mathcal{L}_2$ and $\mathcal{L}_3$ into the loss function, which enables to train the AE being inner and lossless information compression.

- It is noteworthy that the role of the latent variable in approaching the optimal fault detection solution is of indispensable importance. The latent variable can be interpreted as a minimal sufficient statistic in the information theoretic framework. Moreover,

- the I-AE based optimal fault detection system is realized in the data-driven fashion without process models and analytical solutions of (partial) differential equations.

We would like to mention that in the experiments, possible impacts of NN types and structures on AEs and fault detection systems have not been in the focus of our investigation. It can be expected that further improvement of fault detection performance could be achieved by targeted selection of NN types and structures, in particular when complex nonlinear dynamic systems are under consideration. Furthermore, in our study, the threshold setting has been realized in a simple and straightforward way. Also in this regard, improvement of fault detection performance can be expected, for instance, applying the probabilistic threshold setting methods (Xue et al., 2020).

### 5 Conclusions

In this paper, an AE-based solution of optimal fault detection in nonlinear dynamic systems has been studied and validated. As often demanded in engineering applications, optimal fault detection is hereby formulated as maximal fault detectability subject to FAR requirement. Dynamic systems considered in this work differ from those objects and processes addressed by the existing AE-based fault (anomaly) detection and classification methods generally in their complex dynamics and corrupted hybrid uncertainties. In control theory, there exist, on the one hand, well-established methods to deal with such issues. On the other hand, their application to system design and optimization requires the existence of analytical process models and solutions of (partial) differential equations. The basic idea of this work is to fuse the learning capability of NNs and AEs and rich control theoretic knowledge to approach optimal fault detection in nonlinear dynamic systems in the data-driven and learning fashion.

In the first part of our work, the coprime factorization technique has been applied to the establishment of a fault detection framework, including SIR and image subspace for LTI models, orthogonal projection onto system image subspace and optimal fault detection system design. In this regard, the concepts of latent variable for LTI systems and lossless information compression have been introduced. On the basis of Hamiltonian system theory, these results and concepts have been extended to nonlinear dynamic systems. It has been proven that a nonlinear SIR system results in lossless information compression and delivers an optimal fault detection solution if it is inner.

Guided by the aforementioned control theoretic results, an AE-based optimal fault detection system has been realized and validated. The core of this part of our work is the control theoretically explained training of the AE. To be specific, two regularized terms have been added
in the loss function, which results in the so-called I-AE, an AE that is inner. It has been validated that the latent variable in the I-AE is lossless information compression. A comprehensive data experimental study on the laboratory TTS20-simulator has impressively demonstrated that

- the experimental results conform with the theoretic results, namely, the I-AE-based fault detection system increases fault detectability considerably in comparison with a standard AE-based detection system, while satisfying the FAR requirement,
- by means of the I-AE, the optimal fault detection system is realized by learning in the data-driven fashion without process models and analytical solutions of (partial) differential equations,
- learning the latent variable being lossless information compression is of indispensable importance to approach the optimal fault detection solution.

In parallel to the aforementioned investigations, information theoretic aspects of the proposed I-AE have been studied as well. Inspired by the discussion on information bottleneck in the context of feature learning, in particular the concept of minimal sufficient statistic as an optimal latent variable, information relations between the process data and latent variable have been analyzed by means of mutual information rate. It has been proven that, on assumption of the defined system model setting, the mutual information rate of process data and latent variable is zero. This result implies that (i) the latent variable is a minimal sufficient statistic and contains no uncertainties corrupted in the collected process data, and thus (ii) the maximal fault detectability can be achieved thanks to the maximal sensitivity of the evaluation function to the faulty operations.

Our near future work will be devoted to the application study on complex nonlinear dynamic systems and the extension to fault isolation and classification. In course of this work, also research efforts will be made on (i) impact analysis of NN types and structures on fault diagnosis performance, and (ii) threshold setting in the probabilistic framework.

**Acknowledgement:** The authors are grateful to Dr. D. Zhao for the intensive and valuable discussions.

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