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Prognostics and Health Management (PHM): where are we and where do we (need to) go in theory and practice Enrico Zio

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9 ABSTRACT

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11 We are performing the digital transition of industry, living the 4th industrial 12 revolution, building a new World in which the digital, physical and human dimensions are 13 interrelated in complex socio-cyber-physical systems. For the sustainability of these transformations, knowledge, information and data must be integrated within model-based and 14 15 data-driven approaches of Prognostics and Health Management (PHM) for the assessment and 16 prediction of structures, systems and components (SSCs) evolutions and process behaviors, so 17 as to allow anticipating failures and avoiding accidents, thus, aiming at improved safe and 18 reliable design, operation and maintenance.

There is already a plethora of methods available for many potential applications and more are being developed: yet, there are still a number of critical problems which impede full deployment of PHM and its benefits in practice. In this respect, this paper does not aim at providing a survey of existing works for an introduction to PHM nor at providing new tools or methods for its further development; rather, it aims at pointing out main challenges and directions of advancements, for full deployment of condition-based and predictive maintenance in practice.

Keywords: Prognostics and Health Management (PHM), predictive maintenance, Recurrent
 Neural Networks (RNNs), Reservoir Computing (RC), Generative Adversarial Networks
 (GANs), Deep Neural Networks (DNNs), Optimal Transport (OT)

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30 NOMENCLATURE

AAKR	Auto-Associative Kernel Regression
AANN	Auto-Associative Neural Networks
ADNN	Adjacency Difference Neural Network
AE	Auto-Encoder
AE-	
GAN	Auto-Encoder aided GAN
ALE	Accumulated Local Effect
ANNs	Artificial Neural Networks
ARM	Association Rule Mining
ARMA	Auto-Regressive Moving Average
BN	Bayesian Network
CatAAE	Categorical Adversarial Autoencoder
CBM	Condition-Based Maintenance
CDT	Cumulative Distribution Transform
CNN	Convolutional Neural Network
CVNN	Complex Valued Neural Network
DAE	Denoising Auto Encoder

DBN	Deep Belief Network
DL	Deep Learning
DNNs	Deep Neural Networks
DT	Decision Trees
ELM	Extreme Learning Machine
EM	Expectation Maximization
EMD	Earth Mover's distance
ESNs	Echo-State Networks
FCM	Fuzzy C-Means
FFT	Fast Fourier Transform
GANs	Generative Adversarial Networks
GLRT	Generalized Likelihood Radio Test
GRU	Gated Recurrent Unit
HI	Health Indicator
HMM	Hidden Markov Model
ICE	Individual Conditional Expectation
ICT	Information and Communication Technology
IoTs	Internet of Things
KD	Kantorovich distance
KF	Kalman Filtering
KNN	K-Nearest Neighbor
LDA	Linear Discriminant Analysis
LIME	Local Interpretable Model Explanation
LS	Least Square
LSTM	Long Short Term Memory
MAR	Missing At Random
ML	Machine Learning
MODE	Multi-Objective Differential Evolution
NPPs	Nuclear Power Plants
OC-	
SVM	One Class-Support Vector Machine
OT	Optimal Transport
OTT	Optimal Transport Theory
PCA	Principle Component Analysis
PDP	Partial Dependence Plot
PF	Particle Filtering
PFSA	Probabilistic Finite State Automation
PHM	Prognostics and Health Management
PPIs	Prognostic Performance Indicators
RC	Reservoir Computing
KF	Random Forest
KNNS	Recurrent Neural Networks
KUL	Remaining Useful Life
RVM	Relevance Vector Machine
SA	Sensitivity Analysis

SaNSDE	Self-adaptive Differential Evolution with Neighborhood Search
SC	Spectral Clustering
SOM	Self-Organizing Map
SPRT	Sequential Probability Ratio Test
SSCs	Structures, Systems and Components
STPN	Spatio-Temporal Pattern Network
SVM	Support Vector Machine
TOPSIS	Technique for Order of Preference by Similarity to Ideal Solution

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1. INTRODUCTION

35 Prognostics and Health Management (PHM) is a computation-based paradigm that elaborates on physical knowledge, information and data [1] of structures, systems and 36 37 components (SSCs) operation and maintenance, to enable detecting equipment and process anomalies, diagnosing degradation states and faults, predicting the evolution of degradation to 38 39 failure so as to estimate the remaining useful life (Figure 1). The outcomes of the PHM 40 elaboration are used to support condition-based and predictive maintenance decisions for the 41 efficient, reliable and safe operations of SSCs [2]–[5]. In fact, the capability of deploying 42 these maintenance strategies provides the opportunity of setting efficient, just-in-time and 43 just-right maintenance strategies: in other words, providing the right part to the right place at 44 the right time. This opportunity is big because doing this would maximize the production 45 profits and minimize all costs and losses, including asset ones [6]. As a result, in the past 46 decade PHM research and development has intensified, both in academia and industry, 47 involving various disciplines of mathematics, computer science, operations research, physics, 48 chemistry, materials science, engineering, etc. [7], [8].

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52 Figure 1. PHM tasks. The data collected from industrial component sensors feeds 53 three major PHM tasks: fault detection (anomaly detection), fault diagnostics (degradation level assessment) and fault prognostics (remaining useful life prediction). The successful
 deployment of PHM provides solid foundations for the optimal maintenance decisions, and
 thus improve the safety of industrial SSCs while reducing cost.

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58 For making reliability and safety decision using PHM outcomes in practice, 59 identifying, understanding and quantifying the impacts and benefits that the development of a 60 PHM system can have on the health management of a SSC is necessary (e.g. avoid unexpected catastrophic failures, reduce maintenance frequency, optimize spare parts and 61 62 storage, optimize resources, etc.). Then, the practical implementation of PHM includes data 63 acquisition to enable detection, diagnostics and prognostics tasks, and maintenance decision 64 making [9] (Figure 1). The supporting PHM development framework (Figure 2) and its 65 requirements must, then, be properly defined to perform well in real industrial scenarios [9]-[11]. Given the increasing complexity, integration and informatization of modern engineering 66 SSCs, PHM can no longer be an isolated addition for supporting maintenance but must be 67 68 closely linked to the other structure, power, electromechanical, information and 69 communication technology (ICT), control parts of the systems. Then, PHM must be included 70 at the beginning of the system conceptualization, and carried through its design and 71 development in an integrated framework capable of satisfying the overall operation and 72 performance requirements [12], [13].

73 Finally, for the use of PHM in practice, the question of which methods to use is 74 fundamental. For example, referring, in particular, to the prognostic task of PHM, the 75 prediction capability of a prognostic method refers to its ability to provide trustable predictions of the Remaining Useful Life (RUL), with the quality characteristics and 76 confidence level required for making decisions based on such predictions. Indeed, this heavily 77 78 influences the decision makers' attitude toward taking the risk of using the predicted RUL 79 outcomes to inform their decisions [14]. The choice of which method to use is typically 80 driven by the data available and/or the physics-based models available, and the cost-benefit 81 considerations related to the implementation of the PHM system. A set of Prognostic 82 Performance Indicators (PPIs) must be used to guide the choice of the approach to be 83 implemented, within a structured framework of evaluation. These PPIs measure different 84 characteristics of a prognostic approach and need to be aggregated to enable a final choice of prognostic method, based on its overall performance [15]. For this reason, various 85 performance metrics have been defined to enable the evaluation of the performance of PHM 86 87 methods [16]. These metrics are needed to guide the PHM system development (Figure 2). 88



91 *Figure 2 PHM development framework for informed decision-making* 92 93 Up to now, for the maturation of PHM, the main efforts have been mainly devoted to 94 the development of hardware (i.e., Internet of Things (IoTs), smart meters, etc. [17]-[20] and 95 software for tracking the health state of monitored equipment (e.g., data analytics, platforms 96 for IoT interconnection and clouding for computing, etc. [21]–[23]). On the other hand, the 97 full deployment of PHM in practice involves other aspects, including design (e.g. the use of 98 smart components may lead to different reliability allocation solutions), and impacts various 99 work units involved in maintenance decisions and actuations (e.g., workers can use smart

systems, maintenance engineers can analyze big data), including the supporting logistics

(spare parts availability and warehouse management can be driven by the PHM results) [17].
In this paper, we present some main challenges for the development of PHM in
practice, corroborated by practical examples, and associate to some of them the developments
of Recurrent Neural Networks (RNNs), Reservoir Computing (RC), Generative Adversarial
Networks (GANs), Deep Neural Networks (DNNs), Optimal Transport Theory (OTT), as
potential directions to successfully address them.

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2. CHALLENGES TO PHM IN PRACTICE

111 Main challenges to the deployment of PHM in practice still remain, coming from 112 different sides:

- the physics of the problem
 - the data available
 - the requirements of the solutions.

The challenges related to the physics of the problem derive from the complexity of the SSCs degradation processes, which are not completely known, dynamic and highly nonlinear, and hence their understanding, characterization and modelling are difficult.

119 The challenges related to the data relate to multiple aspects (Figure 3):

- the many anomalies in the real data collected in the field (including missing data and erroneous data from malfunctioning sensors)
 - the scarcity and incompleteness of data recognizably related to the state of degradation of the SSC of interest (labelled patterns)
- the difficulty of managing and treating big data, with a large variety of signals collected by sensors of different types
- the changing operational and environmental conditions which affect the data used to train the PHM models and calibrate their parameters, and on which the models are applied.



Figure 3 PHM challenges from data. Fault detection is affected by the challenge of missing data and erroneous data from malfunctioning sensors; fault diagnostics is affected by the challenge of missing labels relating to the state of degradation of the SSCs; fault prognostics is affected by the challenge that data are collected in event-based scenarios because of the difficulty of managing and treating big data.

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138 The challenges related to the requirements of the PHM solutions come from the 139 multiple objectives that they must achieve, depending on the applications. The obvious ones 140 are accuracy and precision, quantified with defined performance indicators and measured 141 against the decisions that they support: in some cases, very high accuracy and precision is 142 required to be able to take confident decisions (e.g. of stopping a system upon an alert of fault 143 detection, of replacing a component upon a fault diagnosis, of anticipating or postponing a 144 scheduled maintenance based on accurate remaining useful life predictions); in other cases, 145 accuracy and precision need not be so high, and may be compromised for other objectives. 146 For example, transparency, explainability and interpretability of PHM models are attributes of 147 particular interest, if not demanded, for decision making in safety-critical applications, for 148 which they may also be a regulatory prerequisite. Also, PHM as a data-dependent enabling 149 technology for smart condition-based and predictive maintenance has issues regarding 150 security. Indeed, the technological network supporting PHM is made of devices, 151 communication technologies and various protocols, so that security issues regarding 152 availability, data integrity, data confidentiality and authentication exist. As these issues 153 hamper operational efficiency, robustness and throughput, they must be adequately addressed.

154 Finally, an enveloping challenge to the deployment of PHM in practice comes from 155 the fact that the PHM tasks of fault detection, diagnostic and prognostic are inevitably 156 affected by various sources of uncertainty, such as incomplete knowledge on the present state 157 of the equipment, randomness in the future operational usage profile and future evolution of 158 the degradation of the equipment, inaccuracy of the PHM model and uncertainty in the values 159 of the signal measurements used by the PHM model to elaborate its outcomes, etc. Therefore, 160 any outcome of a PHM model should be accompanied by an estimate of its uncertainty, in order to confidently take robust decisions based on such outcome, considering the degree of 161 162 mismatch between the PHM model outcomes and the real values.

As these issues hamper operational inefficiency, robustness and throughput, they mustbe adequately addressed.

165 With specific reference to data-driven methods and models for the tasks of fault 166 detection, fault diagnostics and failure prognostics in PHM, the next section addresses some of the above challenges with the focus on advanced methods that are proving as promising fortheir solution.

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3. ADVANCING METHODS OF FAULT DETECTION, FAULT DIAGNOSTICS AND FAILURE PROGNOSTICS FOR MEETING THE CHALLENGES OF PHM IN PRACTICE

174 Methods of fault detection, fault diagnostics and failure prognostics within the PHM 175 framework are continuously being developed and advanced, and applications to various SSCs 176 are being deployed, supported by the technology of sensors and monitoring systems, the techniques of data analytics, image processing and text mining, mostly based on the Artificial 177 178 Intelligence (AI) and Machine Learning (ML) paradigms, and the computational power [24]. 179 The objective of fault detection is to recognize abnormaities/anomalies in SSCs behavior. The 180 objective of fault diagnostics is to identify the SSCs degradation states and the causes of 181 degradation. Prognostics aims at predicting the SSCs Remaining Useful Life (RUL), i.e. the 182 time left before it will no longer be able to perform its intended function. Fault detection and 183 diagnostics, and failure prognostics are the enablers of condition-based and predictive 184 maintenance, which offers major opportunities for Industry 4.0 and smart SSCs, as they can allow reducing failures, increasing SSCs usage, and reducing operation and maintenance 185 186 costs, with tangible benefits of reduction of production downtime, risk and asset losses, and 187 consequent increase of production profit [24].

A number of challenges still remain, arising from the complexity of the physics which PHM is addressed to in practice, from the data available and from the requirements to the PHM solutions for practical applications. In this Section, we go through some of these challenges, to see where we stand, and where we are going and need to go.

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3.1 Data Challenges

3.1.1 Fault detection

195 As mentioned above, fault detection is the PHM task which aims at identifying the 196 presence of abnormalities/anomalies during the operation of a SSC. While such 197 abnormalities/anomalies are commonly referred to as faults in certain disciplines, such as 198 energy and mechanical engineering, the term damage is commonly used in some other 199 disciplines such as structural engineering. In practical applications, fault/damage detection is 200 challenging because it is necessary to assess the presence of the fault/damage based on signals 201 of physical variables measured during the SSC operation and such process is complicated by 202 the various sources of uncertainty that can render the signal processing extremely difficult.

203 Fault detection methods are classified as model-based and data-driven [25]. Model-204 based methods use first principles and physical laws to describe the physical phenomena and 205 processes of interest [26][27][28]. For example, [26] builds a model of the behavior of a rotor 206 using the finite element method and successfully applies it to fault detection. [27] introduces a 207 model-based fault detection and isolation technique for manufacturing machinery based on a 208 defined relationship between a fault signal and observer theory. [28] presents a two-level 209 Bayesian approach based on the use of Hidden Markov Model (HMM) and Expectation 210 Maximization (EM) to detect early faults in a milling machine. However, the practical application of model-based methods is limited by the difficulty of developing accurate 211 212 mathematical models of the processes and behaviors of complex modern SSCs [29].

For this reason, data-driven fault detection methods are more popular than modelbased ones, as they rely only on data for the recognition of anomalous patterns attributable to faults [30][31][32][33][34][35]. For example, [30] develops a fault detection method for power generation systems, by combining Principle Component Analysis (PCA) for feature 217 extraction and Random Forest (RF) for fault behavior pattern learning. Support Vector 218 Machine (SVM) techniques are introduced to detect faults considering concept drift in nuclear 219 power plants [31], and to detect faults in high speed train brake systems in case of highly 220 imbalanced data [35]. Neural Network based approaches attract attention in fault detection, 221 e.g. [32] combines a set of Artificial Neural Networks (ANNs) through Bayesian statistics for 222 heavy-water nuclear reactor fault detection and uncertainty quantification, [34] uses ANN to 223 detect false alarms in wind turbines for reliability centered maintenance, [33] introduces a 224 Recurrent Neural Network (RNN) with optimized hyperparameters for the detection of 225 software faults.

These methods can be divided in those which rely on one-class classification models and those which use residuals, i.e., the differences between the real measurements and the reconstructed values of the signals in normal conditions, to identify the normal/abnormal conditions [36].

230 The former require training of a one-class classification model on signal 231 measurements collected from both normal (healthy) and abnormal/anomalous (faulty) 232 conditions of SSCs. However, in practical applications, faults are rare and the data have 233 manifold distributions embedded in high-dimensional spaces. Distributions with non-smooth 234 densities and the curse of dimensionality of the data in the long-term multivariate time series collected from sensors on real industrial SSCs, can cause model overfitting and render 235 236 difficult the empirical reconstruction of the data distribution, which, therefore, leads to unsuccessful detection of abnormal/anomalous conditions in SSCs behavior. These technical 237 238 issues hamper the successful deployment of one-class classification methods for fault 239 detection in practical applications. The need is, then, to develop methods able to detect anomalous (faulty) conditions given data in normal conditions, and to deal with the manifold 240 241 distribution and large dimensionality of real data. In this direction, Generative Adversarial 242 Networks (GANs) are an interesting perspective as they can be used to reproduce complex distributions, e.g. manifolds [37], [38]. An example is given in the work by [39], which 243 244 proposes an Auto-Encoder aided GAN (AE-GAN) model for the detection of 245 abnormal/anomalous conditions in the behavior of a SSC, in which the generator of the GAN 246 and an auxiliary encoder form an AE module, and the reconstruction error generated by the 247 AE is used as score to detect abnormalities/anomalies in the SSC behavior. Adaptive noise is 248 added on the data and AdaBoost ensemble learning is adapted to integrate the AE-GANs 249 applied to detect anomalies in each small time slice of the long-term multivariate time series 250 collected by the sensors [40]. Furthermore, this work derives a lower bound of Jensen-251 Shannon divergence between generator distribution and normal data distribution as an 252 objective to optimize the AE-GANs hyperparameters; by probing, the optimization works 253 without test data, as commonly needed by other methods. Extensive experiments are 254 conducted on real industrial datasets to demonstrate the usefulness of the developed Adaboost 255 ensembled AE-GAN method for abnormality/anomaly detection in practice.

Residual-based fault detection methods rely on the use of normal-conditions (healthy) 256 257 data, only [41]. These methods reconstruct the values of the signals expected in normal 258 conditions and use the residuals, i.e., the differences between the real measurements and the 259 reconstructed signals, to identify the normal/abnormal conditions. Examples of residual-based 260 methods include Auto-Associative Kernel Regression (AAKR) [42]-[44], Principal Component Analysis (PCA) [45], One Class-Support Vector Machine (OC-SVM) [46], and 261 Artificial Neural Networks (ANNs) [47]. The empirical model, fitted to the data so as to 262 263 provide accurate signal reconstructions, plays an essential role in the above procedure. However, its training may require a large amount of healthy data collected under various 264 265 operating conditions [48]. Besides, different choices of the reconstruction model may yield 266 different detection results [49].

Eventually, the detection of an abnormal condition is confirmed by considering 267 whether the obtained residuals exceed a threshold or by statistical tests. For example, [43] 268 269 uses the Sequential Probability Ratio Test (SPRT) on the residuals obtained from an AAKR 270 model; [50] applies T2- and Q-statistics of the PCA residuals to detect damages in structures; 271 [51] establishes a statistical hypothesis model in the residual subspace of PCA transform, to 272 detect and isolate sensor faults based on a Bayesian formulation and the generalized 273 likelihood radio test (GLRT). Notice that, although these methods assume a certain 274 distribution of the residuals, most distributions of real-world data may be a priori unknown or 275 may not actually follow the assumed distributions [52].

Another challenge of fault detection lies in the data pre-processing [53] to extract features providing the information useful for enabling the detection. Various pre-processing techniques, such as Fast Fourier Transform (FFT) [54], Continuous Wavelet Transform [55], Mathematical Morphology [56], have been applied to raw signals, and the processed outcomes have been fed to fault detection [57]. The quality of the features selected by preprocessing strongly impacts the detection results, but unfortunately there is no universal rule for choosing the optimal pre-processing method.

Recently, transport-related methods are being considered for applications in PHM. They have already been successfully employed in other domains [58], involving signal and image processing [59], computer vision[60], machine learning and statistics [61], [62]. Commonly used optimal transport distances include Wasserstein distance (or Kantorovich distance) [63] and Earth Mover's distance (EMD) [64]. Wasserstein distance has proved a promising statistic for the nonparametric two-sample test [65].

289 In the PHM area, [66] has studied the bearing diagnostics problem using EMD 290 combined with dynamical system reconstruction. [67] has used a PCA scheme combined with 291 the Kantorovich distance (KD) for fault detection in the process industry. [68] has developed a 292 method of OT in which the abnormality score is built using the Wasserstein distance and has 293 verified its performance considering the detection of abnormal conditions in bearings. The 294 method differs from other state-of-the-art methods for fault detection, since it directly deals 295 with raw signals and does not require the use of signal reconstruction methods or feature 296 extraction; it is also distribution-free, i.e., it does not require to formulate any a priori 297 hypothesis on the distribution of the data. The basic idea behind the method is to generate an 298 abnormality score, based on Wasserstein distance, to quantify the dissimilarity between the 299 probability distributions of the currently monitored and healthy data. The Cumulative 300 Distribution Transform (CDT) [69] is used to find the univariate Optimal Transport (OT) 301 solution. The method has been applied to a real bearing dataset and successfully compared 302 with two other fault detection methods of literature: a Z-test based method [70] and a PCA-303 based method for signal reconstruction, combined with the O-statistic for residual analysis 304 [71]. The Adaboost ensembled AE-GAN method mentioned earlier [39] can also be adapted 305 for application to normal-conditions data only. The generator of the GAN and the auxiliary 306 encoder form the AE module, and the reconstruction error generated by the AE is used as the 307 score to detect abnormalities/anomalies in SSC behavior. For the abnormality/anomaly 308 detection, it is assumed, as usual, that the probability distribution of the abnormal/anomalous-309 conditions data is significantly different from that of the normal-conditions data: as the 310 generator can only reproduce the distribution of the normal-conditions data, the AE always 311 successfully reconstruct the normal data but fails to reconstruct the abnormal ones. So, any 312 test sample processed through the AE-GAN is declared anomalous if the AE reconstruction 313 error is larger than a certain predefined threshold. For dealing with the high dimensionality of the data, again, an ensemble framework can be used. Non-overlapped sliding time windows 314 315 are introduced to partition the multivariate time series and a separate data sample for each 316 time window is analyzed by AE-GAN for abnormal/anomaly detection. Finally, the AdaBoost 317 algorithm is used to aggregate the abnormality/anomaly detection results for each time 318 window. The GAN-based method for addressing the challenge of missing fault data in fault

window. The GAN-based method for addressing the challengedetection is shown in Figure 4.

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322Figure 4 Illustration of GAN-based method in fault detection w.r.t. the challenge of
missing fault data [39]. GAN-based method is a type of distribution reconstruction method
which reproduces the normal-conditions data distribution by the Generator and uses an extra
Encoder to form an Auto-Encoder, which can obtain anomaly scores (reconstruction errors)
to distinguish whether samples are anomalous or not.

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Table 1 summarizes the fault detection techniques, with specific regard to the challenge of missing fault data.

330	Table 1 Fault de	tection technique	s with regard to	the challenge of	⁻ missing fault data.
		•	5	5	0

Model-based	Data-driven				
	Supervised	One-	One-class classification		
	learning	(Advantage: address	sing the challenge	of missing fault	
	(Limitation: need		data)		
	both healthy and	Residual-based	Transport-	Distribution	
	fault condition	(Limitation: need	related	reconstruction-	
	data)	to apply statistical		based	
		test)			
Finite	RF:	AAKR: EMD: GAN-based		GAN-based:	
Element	[30] power	[42] non-linear	[66] bearing	[39] high-	
Method:	generators fault	multimode fault detection speed trai		speed train	
[26] rotor	detection	processes fault automatic		automatic door	
crack		detection			
oraon		detection			
diagnostics		detection [43] reactor coolant			
diagnostics		detection [43] reactor coolant pump fault detetion			

		fault detection	
Observer	SVM:	PCA:	Kantorovich
theory:	[31] early fault	[45] air handling	Distance:
[27] rotor fault	detection of	unit fault detection	[67] tank
detection	numerical case		heater
	[35] high-speed		simulation
	train brake fault		case fault
	detection		detection
HMM:	ANN:	OC-SVM:	Wasserstein
[28]	[32] heavy-water	[46] building air	Distance:
mechanical	reactor early fault	conditioning	[68] bearings
equipment	detection	system fault	fault detection
early fault	[34] wind turbine	detection	
detection	false alarm		
	detection		
	RNN:	ANN:	CDT:
	[33] software fault	[47] wind turbine	[69] numerical
	detection	gearbox fault	case
		detection	

3.1.2 Fault diagnostics

333 Fault diagnostics requires data analytics capable of identifying the equipment fault state, mode, location and other characteristics of interest, based on monitored signals 334 335 (temperature, pressure, current, acceleration, etc.). As for the detection task previously discussed, in practical applications it also suffers from the presence of uncertainty coming 336 337 from the processing of data of the measured signals. Common approaches make use of 338 historical operational data to build empirical classifiers capable of discriminating different 339 classes from the data, for fault diagnostics. Different classification techniques, such as 340 Complex Valued Neural Network (CVNN) [72], Deep Belief Network (DBN) [73], Bayesian 341 Network (BN) [74], Decision Trees (DT) [75], Linear Discriminant Analysis (LDA) [75], K-Nearest Neighbor (KNN) [75], Artificial Neural Networks (ANNs), Support Vector Machines 342 343 (SVMs) [76][75][77], have been successfully used in applications of different industrial and 344 civil sectors [78]. These methods rely on supervised learning of labelled data, which, 345 however, are rarely available in practice, so that their real application is limited [79]: the real 346 application calls for unsupervised learning of unlabeled data.

347 Unsupervised learning is an important topic in machine learning for time series segmentation [80], [81] and pattern recognition [21], [82], [83]. In fault diagnostic 348 349 applications, it is used to provide abstract representations of the raw measurement data and 350 obtain various clusters representing healthy and faulty conditions [22], [84]–[86]. In the work 351 of [22], a Categorical Adversarial Autoencoder (CatAAE) has been proposed for unsupervised 352 learning aimed at fault diagnostics of rolling bearings. In the work of [84], a diagnostic 353 methodology based on unsupervised Spectral Clustering (SC) combined with fuzzy C-means 354 (FCM) has been developed for identifying groups of similar shutdown transients performed 355 by a nuclear turbine. In [85], Self-Organizing Map (SOM) has been used for clustering and identifying degradation states of a railway-signal system. In [86], a methodology combining 356 357 k-means and Association Rule Mining (ARM) has been developed to mine failure data and 358 diagnose interconnections between failure occurrences in wind turbines. Representation 359 learning can disentangle the different explanatory factors of variation behind the data, making it easier to extract and organize the discriminative information when building fault diagnostic 360 361 models [87]–[92]. In traditional unsupervised methods for fault diagnostics, the features are

362 extracted applying ad hoc signal processing techniques to the collected signals, e.g. Fourier spectral analysis and Wavelet transformations [93]. The processing is heavily dependent on a 363 priori knowledge and diagnostic expertise [22], [94], and can be quite time consuming and 364 365 labor-intensive [88]. Since representation learning is adaptively capable of learning features 366 from raw data, it can constitute an excellent a priori choice for the development of diagnostic 367 techniques. In the work of [95], an unsupervised sparse filtering method based on a two-layer 368 neural network is used to directly learn features from mechanical vibration signals. In the 369 work of [96], a Spatio-Temporal Pattern Network (STPN) based on Probabilistic Finite State 370 Automation (PFSA) and Markov machines is proposed to represent temporal and spatial 371 structures for fault diagnostics in complex systems. However, these conventional 372 representation learning methods cannot capture long-term temporal dependencies in the time 373 series and they typically require high computational complexity.

374 From the above, it is seen that traditional fault diagnostic approaches typically require 375 the acquisition of signal measurements from SSCs whose true degradation state is known. 376 However, to acquire such labelled data is a difficult, expensive and labor-intensive task. 377 Furthermore, streaming data collected in online-monitored SSCs have long-term temporal 378 dependencies. However, unsupervised learning methods have a hard time dealing with long-379 term time dependencies, because these dependencies are limited by the size of the sliding time 380 window which can be used for the analysis. Then, there is a need for advancements in the 381 methods to estimate the degradation level at a given time on the basis of a few run-to-failure 382 trajectories with long-term temporal dependencies and for which the true degradation state is 383 unknown. In the work of [97], for example, a two-stage method for unsupervised learning is 384 proposed for fault diagnostic applications, inspired by the idea of representing temporal 385 patterns by a mechanism of neurodynamical pattern learning, called Conceptor. Considering a 386 reservoir, i.e. a randomly generated and sparsely connected RNN [98], Conceptors can be 387 understood as filters characterizing the geometries of the temporal states of the reservoir 388 neurons in the form of square matrices [99], achieving a direction-selective damping of high-389 dimensional reservoir states [100]. The proposed method develops in two stages. In the first 390 stage, the Conceptors extracted from the training run-to-failure degradation trajectories are 391 clustered into several non-overlapped time series segments representing different degradation 392 levels. In the second stage, the Conceptors and corresponding labels obtained in the first-stage 393 clustering are used to train a Convolutional Neural Network (CNN) for real-time diagnosing 394 the SSC degradation level. The CNN receives in input the Conceptors extracted from the 395 reservoir states at the current time, which contain information about the long-term evolution 396 of the SSC degradation, and the difference between the Conceptors extracted at the present 397 and previous time steps, which contains information about the short-term degradation 398 variation. The proposed method has been applied to two literature case studies concerning 399 bearings fault diagnostics. The results show satisfactory accuracy and efficiency of the method. The Reservoir computing-based method for addressing the challenge of missing 400 401 labels of degradation state is shown in Figure 5.



403 Figure 5 Illustration of Reservoir Computing-based method in fault diagnostics w.r.t. 404 the challenge of missing labels of degradation state [97]. a) Conceptor Generator converts 405 the variable-length signals into a fixed-size Coceptor matrix by using reservoir computing. 406 *The Conceptor matrix is a filtered correlation matrix of reservoir states, which decreases the* 407 impact of less important features in the degradation dynamics, i.e. noise and operation 408 conditions. b) stage 1: the combined use of Coceptors matrix and spectral clustering can 409 obtain the pseudo-labels in the run-to-failure trajectories, stage 2:CNN trained by Conceptors 410 with associated pseudo-labels is, then, used for fault diagnostics.

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413 Table 2 summarizes the fault diagnostics techniques, with specific regard to the 414 challenge of missing labels for degradation states.

415 Table 2. Fault diagnostics techniques with regard to the challenge of missing labels for

416 degradation state.

Supervised classifiers	Unsupervised approaches			
(Limitation: need	Unsupervised	Representati	on learning	
degradation state labels)	learning	Neural Network-	Reservoir	
	(Limitation: depend	based	Computing-based	
	on diagnostic	(Limitation:		
	expertise for feature	difficult to capture		
	extraction)	long-term temporal		
		dependencies)		
CVNN:	CatAAE:	Unsupervised	Conceptor + SC:	
[72] railway track	[22] rolling bearing	Sparse Filtering	(Conceptor as a	
turnouts degradation	fault diagnosites	Neural Network:	representation	
level assessment		[95] motor bearing	capable of	
DBN:	SC + FCM:	fault diagnostics	encoding long-	
[73] aircraft engine	[84] Nuclear Power		term temporal	

health state classification	Plant (NPP) steam turbine transient		<i>dependencies)</i> [97] degradation
	identification		level assessment
BN:	SOM:	STPN:	of bearings
[74] failure type	[85] fault mode	[96] fault severities	
classification of water	classification for	diagnostics of wind	
distribution system	railway monitoring	turbine	
	equipment		
DT:	k-means + ARM:		
[75] anomaly (mud)	[86] failure cause		
diagnostic on wind	and weather		
turbine blade	condition correlation		
LDA:	diagnostics of wind		
[75] anomaly (mud)	turbine system		
diagnostic on wind			
turbine blade	-		
KNN:			
[75] anomaly (mud)			
diagnostic on wind			
turbine blade	-		
ANNs:			
[101] fault diagnostics of			
bearings	-		
SVMs:			
[75] anomaly (mud)			
diagnostic on wind			
turbine blade			
[76] bearing defects			
diagnostics			
[//] pipe failure			
prediction in water			
supply networks			

418

3.1.3 Fault prognostics

419 Prognostics is concerned with the prediction of the future evolution to failure of the 420 state of a SSC. It involves the processing of data to predict the future degradation of the SSC 421 structural and functional attributes, based on which to estimate the SSC failure probability and 422 RUL. The prognostic outcomes are used for the health management of the SSC, which seeks 423 to use the prognosis to decide on and actuate operational actions and maintenance 424 interventions. To the uncertainties coming from the use of the data available from the sensors, like for the detection and diagnosis tasks, prognostics adds further challenges related to the 425 426 future evolution of the usage profile and operational environment, whose uncertainties affect 427 the degradation state evolution. This makes it practically impossible to precisely predict the 428 future evolution of the SSC state of health and it is necessary to account for the different 429 sources of uncertainty that affect prognostics, within a systematic framework for uncertainty 430 quantification and management [102].

431 Prognostics is dependent on the available knowledge, information and data on the
432 process of degradation. There may be situations in which a sufficient quantity of run-to-failure
433 data has been collected during the life of the SSCs, and these can be used to develop empirical
434 (data-driven) models. In other cases, the degradation mechanism is known and a physics-

based model is available. On these bases, prognostics approaches can be grouped into threecategories: (i) model-based, (ii) data-driven and (iii) hybrid:

- 437 (i) Model-based approaches use physics-based degradation models to predict the future evolution of the SSCs degradation state and infer the time at which the 438 439 degradation will reach the failure threshold. These approaches have been applied with 440 success in various practical cases, e.g., to pneumatic valves [103], Li-Ion batteries 441 [104], the residual heat removal subsystem of a nuclear power plant [105], and 442 structures subject to fatigue degradation [106]. In the case of complex SSCs, subject to 443 multiple and competing degradation mechanisms, accurate physics-based models are, 444 however, often not available.
- 445 • (ii) Data-driven approaches directly extract from the data the degradation law for SSCs RUL prediction [107]. Such approaches include conventional numerical time series 446 447 techniques, as well as AI intelligence and data mining algorithms, such as similarity-448 based [108] and regression-based methods [107]. A variety of AI techniques, such as 449 Convolutional Neural Network (CNN) [109][110], Denoising Auto Encoder (DAE) 450 [111], Long Short Term Memory (LSTM) [112][109][113][114], Gated Recurrent Unit 451 (GRU) [115], SVM [116], Adjacency Difference Neural Network (ADNN) [117], are 452 applied to RUL estimation of different industrial systems and components. The 453 performances of data-driven approaches depend on the quantity and informative 454 quality of the data available to develop the predictive models.
- (iii) Hybrid approaches combine, all the available sources of knowledge, information 455 456 and data. They bring the advantages of both model-based and data-driven methods. Specifically, they can integrate the robustness and interpretability of model-based 457 458 methods with the specificity and accuracy of data-driven methods. For instance, [118] 459 combines Kalman Filtering (KF) with data-driven approaches, [119] integrates the 460 Health Indicator (HI) and regression model, [120] combines Relevance Vector 461 Machine (RVM) and Particle Filtering (PF), and [121] integrates a physical model and 462 the Least Square (LS) method to estimate RUL of a variety of industrial equipment.

463 Traditional fault prognostic methods face the challenge of dealing with incomplete and 464 noisy data collected at irregular time steps, e.g. in correspondence of the occurrence of 465 triggering events in the system. For example, for monitoring the degradation and failure 466 processes of bearings in large turbine units, signal measurements collection (e.g., vibration 467 signals measured by eddy current displacement sensors measuring the radial vibration of the 468 rotor at both ends, the axial vibration of the rotor, and sensors measuring the unit rotating 469 speed) is only triggered by abnormal behaviors of the units, such as large environmental noise 470 and anomalous vibration behavior. These "snapshot" datasets are often encountered in 471 industrial applications, dominated by the necessity of cost saving in storing and managing the 472 databases, and of reducing energy consumption and bandwidth resources. Since failure events 473 are rare, event-based datasets are dominated by missing measurements, where the values of all 474 signals are missing at the same time. With these characteristics, traditional methods for 475 missing data management, e.g. case deletion, imputation [122]-[125] and maximum 476 likelihood estimation [126], are difficult to apply. For instance, since case deletion methods discard patterns whose information is incomplete, they are not useful in case of event-based 477 datasets where a pattern is either present or absent for all signals [126]. Imputation 478 479 techniques, which are based on the idea that a missing value of a signal can be replaced by a 480 statistical indicator of the probability distribution generating the data, such as the signal mean value [127] or a value predicted by a multivariable regression model, have been shown 481 482 inaccurate in case of large fractions of missing values in the dataset [128]. Maximum 483 Likelihood methods use the available data to identify the values of the probability distribution 484 parameters with the largest probability of producing the sample data. They typically require the Missing At Random (MAR) assumption, i.e. the probability of having a missing value isnot dependent on the missing values[127],[129], which is not met in event-based datasets.

487 Few research works have considered fault prognostics in presence of missing data. A 488 model based on Auto-Regressive Moving Average (ARMA) and Auto-Associative Neural 489 Networks (AANN), has been developed for fault diagnostics and prognostics of water process 490 systems with incomplete data [130]. An integrated Extreme Learning Machine (ELM)-based 491 imputation-prediction scheme for prognostics of battery data with missing data [125] and an 492 hybrid architecture of physics-based and data-driven approaches have been proposed to deal 493 with missing data in a rotating machinery prognostic application [131]. In the medical field, a 494 Bayesian simulator has been used to generate missing data for developing prognostic models 495 [132] and a Multiple Imputation approach has been embedded within a prognostic model for 496 assessing overall survival of ovarian cancer in presence of missing covariate data [133]. 497 Notice that all these methods are based on the two successive steps of missing data 498 reconstruction and prediction.

499 Then, advancements and new methods are still needed to enable predicting the RUL of a 500 SSC on the basis of measurements collected only when triggering events occur, such as SSC 501 faults or extreme operational conditions, and providing an estimate of the uncertainty 502 affecting the RUL prediction. As an example, [134] has developed a method based on Echo-503 State Networks (ESNs) to directly predict the RUL of a SSC without requiring to reconstruct 504 the missing data. ESNs are considered because of their ability of maintaining information 505 about the input history inside the reservoir states. The main difficulty is that, contrarily to the 506 typical applications of ESNs, the time intervals at which the data become available are 507 irregular. Two different strategies have been considered to cope with the event-based data 508 collection. In one strategy, the ESN receives an input pattern only when an event occurs. The 509 pattern is formed by the measured signals and the time at which the event has occurred. In a 510 second strategy, the reservoir states are excited at each time step. If an event has occurred, the 511 reservoir states are excited both by the previous reservoir states and the measured signals, 512 whereas, if an event has not occurred, they are excited only by the previous reservoir states. 513 By so doing, the connection loops in the reservoir allow reconstructing the SSC dynamic 514 degradation behavior at those time steps in which events do not occur. Multi-Objective 515 Differential Evolution (MODE) algorithm based on a Self-adaptive Differential Evolution 516 with Neighborhood Search (SaNSDE) [135] is used to optimize the ESN hyper-parameters. 517 The Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) [136] is, 518 then, used to select the optimal solution from the obtained Pareto solutions. Furthermore, a 519 bootstrap aggregating (Bagging) ensemble method is applied to improve the RUL prediction 520 accuracy and estimate the RUL prediction uncertainty. Given that ESNs cannot be fed by 521 random sequences of patterns, the traditional Bagging sampling mechanism used to create the 522 bootstrap training sets has been modified. In the proposed solution, the bootstrap training sets 523 are obtained by concatenating entire run-to-failure trajectories, randomly sampled with 524 replacement. The benefits of the proposed methods are shown by application to the prediction 525 of the RUL of a sliding bearing of a turbine unit. The ESN-based one-step RUL prediction 526 method for the challenge of missing data, i.e., event-based measurements, is shown in Figure 527 6.

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Figure 6 Illustration of ESN-based method in fault prognostics w.r.t. the challenge of missing data, i.e. event-based measurements [134]. The input neurons of ESN are excited to update the 531 532 reservoir state when measurements are available (events are triggered), whereas the input 533 neurons are canceled if data are missing (no events occur) and the reservoir is only updated 534 by the reservoir state at the previous time step and the target signal, which force the reservoir 535 to learn from the historical degradation pattern and the target signal evolution pattern. 536

- 537 Table 3 summarizes fault prognostics techniques, with specific regard to the challenge 538 of missing data, i.e. event-based measurements.
- 539

540	Table 3. Fault prognostics techniques with regard to the challenge of missing data, i.e. event-
541	based measurements.

Traditional fault prognostics			Fault prognostics in presence of missing	
(Limitations: ca	nnot deal with mi	ssing data, i.e.	data	
event	-based measureme	ents)		
Model-based	Data-driven	hybrid	Conventional type of	Event-based
			missing data	measurement
			(Limitations:	
			difficult to deal with	
			event-based	
			measurements)	
[103] fault	CNN:	KF and	Missing at random	ESN-based
prognostics of	[109] RUL	data-driven	Missing data	one-step RUL
pneumatic	estimation for	approaches:	imputation and	prediction
valves	bearing	[118] RUL	prognostics by	without
[104]	[110] RUL	estimation for	ELM-based	requiring to
prognostics	estimation for	aircraft bleed	method:	reconstruct the
and health	turbofan	valve	[125] RUL	missing data:
monitoring of	engine		estimation of battery	[134] RUL and
Lithium-ion	DAE:	HI and		uncertainty
battery	[111] RUL	regression	Missing not at	estimation of
[105] fault	estimation for	model:	random	bearing

		[110] DUI	Minutes a data	
prognostics in	centriiugai		wiissing data	
residual heat	pumps	estimation for	prediction by	
removal		bearings	Quasi-Newton	
subsystem			Optimization;	
	LSTM:	RVM and	Prognostics by	
	[109] RUL	PF:	AANN and ARMA:	
	estimation for	[120] RUL	[130] prognostics for	
	bearing	estimation for	wastewater plant	
	[112] RUL	Lithium-ion	Missing at extreme	
	estimation for	battery	operating condition	
	turbofan	5	Missing data	
	engine	nhysical	generation hv	
	[113] RUL	model and	nhysical model.	
	estimation for		Prognostics by	
	turbofan		nhysical model and	
	engine	[121] KUL	data drivon.	
		Estimation for	[121] progratics for	
	estimation for	Liunium-ion	[151] prognostics for	
	turbofon	battery	bearing	
	angina			
	engine			
	GRU:			
	[115] RUL			
	estimation for			
	turbofan			
	engine			
	SVM.	1		
	astimation for			
	csumation for			
	aircrait engine	4		
	ADNN:			
	[117] RUL			
	estimation for			
	aircraft engine			

543 544 3.2 Challenges from requirements on practical solutions

3.2.1 Interpretability of models

545 The ability to correctly interpret a PHM model's output, be it the detection of a fault, 546 its diagnosis or prognosis, is extremely important, and particularly so in safety-critical applications like those concerning the high-risk systems and processes of the chemical, 547 548 nuclear, aerospace industries, to name a few. It allows understanding of the state of the system 549 or process being modeled and supports analytic reasoning and prescriptive decision making to 550 intervene (or not) and how. It also engenders appropriate trust by the analyst, providing 551 insights on how the model works. The importance of this is such that in some applications, 552 simple models (e.g., even linear models) are preferred for their ease of interpretation, even if 553 they may be less accurate than complex ones. Yet, currently the growing availability of big 554 data for PHM has increased the benefits of using complex models for achieving accuracy, at 555 the expenses of model intelligibility. This brings to the forefront the need of a trade-off between accuracy of the model and interpretability of its output. A wide variety of different 556

557 methods have been recently proposed to address this issue, but an understanding of how these 558 methods relate and when one method is preferable to another is still lacking.

559 Most models and algorithms for PHM are developed and trained to maximize 560 accuracy, neglecting interpretability and causality. Accounting for these aspects may, indeed, 561 lead to a loss in performance but would enhance their safe, reliable and robust use both in 562 terms of undesired biases and uncertainty reduction. Understanding why a PHM model makes 563 a certain prediction can be as crucial as the prediction's accuracy in many applications. 564 However, the highest accuracy for large modern datasets is often achieved by complex models 565 that even experts struggle to interpret, such as ensemble or deep learning models, creating a 566 tension between accuracy and interpretability [137]. Some general attributes sought for in the 567 interpretability of PHM models are:

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- 569 570

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• robustness: small changes in input should not cause big changes in output

• fairness: no discrimination in algorithm decisions, which could come from bias

- causality: causal relations are picked up from the model and rendered explicit
- quantifiable reliability of outcomes and predictions.

in the collected data

573 The awareness of the relevance of transparency, explainability and interpretability of PHM 574 models is growing as a need and a requirement, particularly for supporting decision making in 575 safety critical systems, for which it may also be a regulatory prerequisite. For example, in 576 Nuclear Power Plants (NPPs), there is still resistance to the deep penetration of digital I&C 577 systems and PHM, because of the difficulty of testing performance under all postulated 578 conditions, on one side, and guaranteeing reliability based on transparent understanding and 579 interpretation, on the other side. The decision making related to tasks of control, operation, 580 maintenance and safety of NPPs, which have traditionally relied on procedures and expert 581 evaluation and judgment, are gradually being assisted by intelligent machines (i.e. software 582 algorithms) for PHM, developed and trained on the basis of big and customized data: how far and how it can be permitted in safety-critical systems that require licensing depends also on 583 584 the possibility of interpreting the causality of their output.

For the modelling approaches to PHM based on learning from data, one issue lies in possible biases in the training set that are, then, not present in the test set or contain patterns undesired with respect to the test data, and may be unknown to the user of the trained model output. In this sense, achieving robustness in PHM models is fundamental and one way to proceed is to try to design inherently interpretable models, i.e. so as to exclude all undesired features that are not causally related to the outcome. By examining interpretable models:

- features or functions capturing quirks in the data can be noted and excluded, thereby
 avoiding related harm in the successive use of the model output, and the understanding
 of the phenomena analyzed
- knowledge can be extracted, in terms of the interactions among the inputs and how
 they determine the output
- an evaluation of the reliability of the PHM outcomes can be performed
- some limited extrapolation can be possible, with the aim of gaining knowledge on unexplored scenarios.

599 Methodologies are used to gain interpretability in a model by looking at the importance of the 600 different input features in determining the model outputs. A distinction is made between 601 model-specific and model-agnostic methodologies for evaluating feature importance. An 602 interesting example of the former is the "attention mechanism" for Neural Networks applied 603 in Prognostics, where importance values are assigned to specific input subsets [138], [139].

604 As the name implies, model-agnostic feature importance evaluation methodologies can 605 in principle be used for any model. Local approaches are used for online applications and 606 global approaches for offline applications. Local measures focus on the contribution of 607 features to a specific outcome instance, whereas global measures take all outcomes into 608 account.

609 The Local Interpretable Model Explanation (LIME) method aims at explaining 610 individual outputs and can be applied to any learning model [140]. Instead of training a global 611 surrogate model, LIME focuses on training local surrogate models to explain individual 612 model outputs. The method works by building for each output instance of interest a local-613 interpretable model that approximates the original, complex model. Each model output instance is, then, explained by an "explainer-model" that highlights the symptoms that are 614 615 most relevant to it. With this information about the rationale behind the model, the analyst is 616 now empowered to trust the model output-or not - for her/his decisions and consequent 617 actions.

618 The idea behind LIME is quite intuitive and it is based on the fact that one can probe 619 the model as many times as desired, by feeding the input data points and retrieving the 620 corresponding outputs of the model. The goal of this is to understand why the learning model 621 gave a certain output. The LIME tests are local sensitivity tests performed in a way to explore 622 what happens to the output when the inputs are locally varied by small perturbations. By so 623 doing, a new dataset is generated, consisting of permuted input samples and corresponding 624 model outputs. For example, the new samples can be created by perturbing each feature individually, drawing from a normal distribution with mean and standard deviation taken from 625 626 the feature values. On this new dataset, LIME builds and trains the interpretable explainer-627 model, which is weighed by the proximity of the sampled instances to the instance of interest. 628 The interpretable model should give a good approximation of the original model outputs 629 locally, but it does not have to be a good global approximation of the original model itself. Mathematically, the interpretable explainer model for instance x is the (simple) model g (e.g. a 630 631 linear regression model) that results as solution of the optimization problem that minimizes 632 the loss function L (e.g. the mean squared error) measuring how close the explanation output 633 of g is to the output of the original model f (e.g. a neural network), while the model 634 complexity $\Omega(g)$ is kept low (e.g. as few features as possible):

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- 636 637

638

$$explanation(x) = argmin L(f, g, \pi_x) + \Omega(g)$$

$$g \in G$$
(1)

639 where *G* is the family of possible explainer models, for example all possible linear regression 640 models, and the proximity measure π_x defines how large is the neighborhood around instance 641 *x* that is considered for the explanation. In practice, LIME only optimizes the loss part and the 642 user controls the model complexity by $\Omega(g)$, e.g. by selecting by forward and backward 643 feature selection methods the maximum number of features that the linear regression model 644 may use.

- 645 The procedure for interpreting locally the complex original model is, then:
- 646 i) select the instance of interest *x* for which an explanation of the original complex model 647 outcome f(x) is needed
- 648 ii) perturb the input data and get the original model output values for these new data649 samples
- 650 iii) weigh the new samples according to their proximity to the instance of interest
- iv) train a weighed, interpretable model on the new dataset generated in *ii*)
- 652 v) explain the local output of the interpretable model *g*.

LIME has been applied for the interpretation of machine learning models in applications of medical diagnostics [141]. In a recent study about early Parkinson detection, LIME has been used to highlight the features determining the healthy/disease decision of a ML classifier of images of the brain: LIME allows highlighting the super-pixels mostly determining the classification in healthy or disease states; experts can, then, focus on the super-pixels selected
with LIME to interpret and explain the basis for the decision by the ML algorithm, and choose
to accept or refuse it.

660 Shapley values also can be used to assess local features importance [142]. Although they 661 can be used to explain which feature(s) contribute most to a specific model output, Shapley 662 values are not designed to answer the "what would happen if" questions that LIME's local 663 explainer models are designed for. They come from game theory and are designed to construct a fair payout scheme for the players in a game. Suppose one could look at all possible 664 665 combinations of (a subset of) players in a team replaying a game and observe the resulting 666 team score. One could, then, assign each player of the team a portion of the total payout based 667 on its average added value across all possible subteams to which it was added to play the 668 game repeatedly. Such individual payout is the player's Shapley value and gives the only payout scheme that is proven to be: 669

- efficient: the sum of the Shapley values of all players should sum up to the total payout
- symmetric: two players should get the same payout if they add the same value in all team combinations
- dummy-sensitive: a player should get a Shapley value of zero if it never improves a subteam's performance when it is added
- additive: in case of a combined payout (say we add two game bonuses), the combined
 Shapley value of a player across the games is the sum of the individual game's
 Shapley values; this criterion has no relevant analogy in the context of model
 interpretability.

In the "game" of our interest for PHM model interpretability, the players are models with different features subsets and they get the same payout mechanism introduced above. The team score in this context is the performance measure of a (sub)model built on a given feature subset. The total payout is the difference between a base value — output of the null model and the actual output. This difference is, then, divided over all features in accordance to their relative contribution.

686 Obviously looking at all possible subsets of features is computationally prohibitive in 687 most realistic models with many features. Instead, Shapley value approximations can be 688 computed based on sampling of features.

689 Other model-agnostic methodologies are based on Sensitivity Analysis (SA), which has 690 been widely applied to models used in various areas, such as nuclear risk assessment [143], 691 industrial bioprocessing [144] and climate change [145]. Indeed, a main application of SA is 692 for identifying the input quantities most responsible of a given output variation [146]. Both 693 local and global approaches to SA have been developed. Local approaches identify the critical 694 input features as those whose variation leads to the most variation in the output. One practical 695 approach for such identification consists in perturbing one single input at a time with small 696 variations around its nominal value, while maintaining the others set at their respective 697 nominal values. The analysis is intrinsically local and the resulting indication can be 698 considered valid for the characterization of the model response around the nominal values. 699 The possibility of extending the results of the analysis to draw global considerations on the 700 model response over the whole input variability space depends on the model itself: if the 701 model is linear or mildly non-linear, then the extension may be possible; if the model is 702 strongly non-linear and characterized by sharp variations, the analysis is valid only locally. Typical local approach techniques are those based on Taylor's differential analysis and on the 703 704 one-at-a-time simulation, in which the input features are varied one at a time while the others 705 remain set at their nominal values [146].

706 In those situations (often encountered in practice) in which models are non-linear and non-707 monotone, the results provided by a local analysis may have limited significance. For this 708 reason, global approaches to SA have been developed. In these approaches, the focus is 709 directly on the uncertainty distribution of the output, which contains all the information about 710 the variability of the model response, with no reference to any particular value of the input 711 (like in the local approaches, where reference is made to the nominal values). The two 712 principal characteristics of the global approaches are somewhat opposite to those of the local 713 ones: 1) the account given to the whole variability range of the input features (and not only to 714 small perturbations around the nominal values); 2) the focus on the effects resulting from 715 considering also the variation of the other uncertain features (instead of keeping them fixed to 716 their nominal values). Many global analysis methods have been developed [146]. The high 717 capabilities of these methods are paid by a very high computational cost.

Another direction to build interpretability into PHM models and algorithms is by integrating prior physical knowledge in the learning models, for providing improved performance and achieving interpretability. This is a promising approach for inducing interpretability into the learning models and different approaches have been proposed where the physical knowledge can be introduced at different levels of the learning process, including in the training data and in the training algorithm [147][148][149][150].

724 To aid the interpretation of the model, there exists also a suite of methods for the 725 visualization of the relations between input and output. The Partial Dependence Plot (PDP) 726 shows the marginal effect that features have on the output provided by the model [151]. 727 Intuitively, we can interpret the partial dependence as the expected target response as a 728 function of the input features of interest. A partial dependence plot can show whether the 729 relationship between the output and a feature is linear, monotonic or more complex. For 730 example, when applied to a linear regression model, partial dependence plots always show a 731 linear relationship. The computation of partial dependence plots is intuitive: the partial 732 dependence function at a particular feature value represents the average output if we force all 733 data to assume that value for the feature. If the feature for which the PDP is computed is not 734 correlated with the other features, then the PDP perfectly represents how the feature 735 influences the output on average. In the uncorrelated case, the interpretation is clear: the PDP 736 shows how the average output changes when a given feature is changed. The interpretation is more complicated when features are correlated. Also, PDPs are easy to implement and the 737 738 calculations to obtain them have a causal interpretation which aids model understanding: one 739 intervenes on a feature and measures the corresponding change in the output. By doing so, 740 one analyzes the causal relationship between the feature and the output in the model, and the 741 relationship is causal for the model whose outcome is explicited as a function of the features. 742 However, there are several disadvantages in PDPs. Due to the limits of human perception, the 743 number of features in a partial dependence function must be small (usually, one or two) and, 744 thus, the features considered must be chosen among the most important ones. Some PDPs do 745 not show the feature distribution. Omitting the distribution can be misleading, because one 746 might overinterpret regions with almost no data. This problem is easily solved by showing a 747 rug (indicators for data points on the x-axis) or a histogram. Also, heterogeneous effects might 748 be hidden because PDPs only show the average marginal effects. Suppose that for a feature, 749 half of the input data has a positive correlation with the output (the larger the feature value the 750 larger the output value) and the other half has a negative correlation (the smaller the feature 751 value the larger the output value): then, PDP could be a horizontal line, since the effects of 752 both halves of the dataset could cancel each other out and one would, then, conclude that the 753 feature has no effect on the output. In other words, whereas the PDPs are good at showing the 754 average effect of the target features, they can obscure a heterogeneous relationship created by interactions. 755

756 When interactions are present, the Individual Conditional Expectation (ICE) plot can be 757 used to extract more insights [152]. An ICE plot shows the dependence between the output and an input feature of interest. However, unlike a PDP, which shows the average effect of the 758 759 input feature, an ICE plot visualizes the dependence of the output on a feature for each sample 760 separately, with one line per sample. Again, due to the limits of human perception, only one 761 input feature of interest is supported by ICE plots. On the other hand, in ICE plots it might not 762 be easy to see the average effect of the input feature of interest. Hence, it is recommended to 763 use ICE plots alongside PDPs: they can be plotted together.

764 Finally, the assumption of independence is the biggest issue with PDPs. It is assumed that 765 the features for which the partial dependence is computed are not correlated with other features. One solution to this problem is Accumulated Local Effect (ALE) plots that work 766 767 with the conditional instead of the marginal distribution (Apley et al., 2020). ALE plots are a faster than and unbiased alternative to PDPs. Based on the conditional distribution of the 768 769 features, they calculate differences in outputs instead of averages. ALE plots are unbiased, 770 which means they still work when features are correlated, and are faster to compute than 771 PDPs. The interpretation of ALE plots is also clear: conditional on a given value, the relative 772 effect on the output due to changing the feature value can be read from the ALE plot. Even 773 though ALE plots are not biased in case of correlated features, interpretation remains difficult when features are strongly correlated. Because if they have a very strong correlation, it only 774 775 makes sense to analyze the effect of changing both features together and not in isolation. This 776 disadvantage is not specific to ALE plots, but a general problem of strongly correlated 777 features. Table 4 summarizes the investigated approaches for interpreting the PHM models.

778 779

Characteristic	Reference
Focuces on training local surrogate	[140]
models to explain individual model	
outputs	
Uses game theory to construct a fair	[137]
payout scheme for the player (input	
features) to obtain features importance	
Identifyies the input quantities most	[143][144][145][146]
responsible of a given output variation	
Builds interpretability into PHM models	[147][148][149][150]
and algorithms by integrating prior	
physical knowledge in the learning	
models	
Shows the average marginal effect that	[151]
features have on the output provided by	
the model	
ICE plots visualize the dependence of the	[152]
output on a feature, for each sample	
separately	
	Characteristic Focuces on training local surrogate models to explain individual model outputs Uses game theory to construct a fair payout scheme for the player (input features) to obtain features importance Identifyies the input quantities most responsible of a given output variation Builds interpretability into PHM models and algorithms by integrating prior physical knowledge in the learning models Shows the average marginal effect that features have on the output provided by the model ICE plots visualize the dependence of the output on a feature, for each sample separately

Table 4 Summary of model interpretability approaches

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782 *3.2.2 Security of models*

Applications of PHM methods for condition-based and predictive maintenance rely on the exchange and elaboration of data. The models and algorithms used are technological elements of larger socio-human-technical systems that must be engineered with safety and security in mind. They are increasingly used in support of high-value decision-making 787 processes in various industries, where the wrong decision may result in serious consequences. 788 The underlying models and algorithms are largely unable to discern between malicious input 789 and benign anomalous data. On the contrary, they should be capable of discerning maliciously-introduced data from benign "Black Swan" events. In particular, the learning 790 791 models and algorithms should reject training data with negative impacts on results. Otherwise, 792 learning models will always be susceptible to gaming by attackers. The specific danger is that 793 an attacker will attempt to exploit the adaptive aspect of a learning model to cause it to fail 794 and produce errors: if the model misidentifies an hostile input as benign, the hostile input is 795 permitted through the security barrier; if it misidentifies a benign input as hostile, the good 796 input is rejected [153]. The adversarial opponent has a powerful weapon: the ability to design 797 training data that cause the learning model to produce rules that misidentify inputs. To avoid 798 this, the models and algorithms used for PHM must have built-in forensic capabilities [154]. 799 These should enable a form of intrusion detection, allowing engineers to determine the exact 800 point in time that an output was given by the model, what input data influenced it and whether 801 or not that data was trustworthy. The data visualization capabilities for the interpretation of 802 the relations between model input features and model output discussed in the previous 803 subsection 3.2.1 show promise to help engineers identify and resolve root causes for these 804 complex issues. Also, specific solutions are required in the areas of Authentication, Input 805 Validation and Denial of Service.

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3.2.3 Uncertainty

808 Uncertainty is intrinsically present in the PHM tasks of detection, diagnostics and 809 prognostics, and may adversely affect their outcomes, so to lead to an imprecise assessment of the state and prediction of the behavior of such systems, which could lead to wrongly 810 811 informed system health management decisions with possibly costly, if not catastrophic, 812 consequences. For practical deployment, it is necessary to be able to estimate the uncertainty 813 and confidence in the outcomes of detection, diagnostics and prognostics activities, for 814 quantifying the risk associated to the PHM decision-making on the operation of engineering 815 systems. Yet, in spite of the recognition of the importance of uncertainty in PHM [155], work 816 is still needed to concretely address the impact of uncertainty on the different PHM tasks and 817 to effectively manage it.

818 The challenge comes from the fact that there are different sources of uncertainty that 819 affect PHM, whose interactions are not fully understood and, thus, it is difficult to 820 systematically account for them in the PHM tasks. While some sources are internal to the 821 SSC, others are external, and all must be accounted for in the different activities of PHM. 822 There is aleatory uncertainty in the physical behavior of the SSC and epistemic uncertainty in 823 the model of it (developed based on sensors data or physic-based or based on a hybrid 824 combination of both data and physics) and the associated parameters. As mentioned earlier, 825 there is uncertainty in the sensors measurements and in their processing tools. For the 826 prognostic task of PHM, there is also uncertainty on the future SSC operation profile and state 827 evolution.

828 Given the relevance of uncertainty in the PHM tasks, it becomes necessary to develop 829 systematic frameworks for accounting for such uncertainty in practical applications, in order 830 to enable the robust verification and validation of the solutions developed, with respect to the 831 requirements for their use for decision-making and their contribution to the risk involved in 832 such decisions. Such frameworks must enable the systematic identification, representation, 833 quantification and propagation of the different sources of uncertainty, so that any PHM 834 outcome is provided also with its uncertainty, which needs to be considered for robust 835 decision-making [156].

836 Focusing specifically on data-driven methods for PHM, the challenge of quantifying 837 the uncertainty in PHM outcomes has rarely been addressed and mostly with ensemble approaches, which can become computationally burdensome, and are highly dependent on 838 839 how the individual models are developed and how their outcomes are aggregated 840 [157][158][159][160][134][161]. Recently, Bayesian neural networks and variational 841 inference have been used in PHM, for accounting of uncertainty [162][163]. Also, the 842 combination of neural networks and gaussian processes are being considered as a promising 843 direction for providing PHM outcomes equipped with the needed estimates of the associated 844 uncertainty [164].

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4. CONCLUSIONS

848 PHM has become a fashionable area of research and development, due to its promises 849 of enabling condition-based and predictive maintenance, which can be game-changers for the 850 production performance, reliability and safety of industrial businesses. Then, many academic 851 words have been and are developed, and several applications have been attempted, with a 852 more or less significant degree of success. These have been facilitated by the availability of 853 numerous and large data sets, of affordable computational hardware to train the models, of 854 freely available software to implement the models in a reliable and relatively straightforward 855 manner. Yet, quite some work still needs to be done to increase the significance of PHM 856 impacts on industry, due to a number of theoretical and practical issues that still require an 857 effective solution. These come from different perspectives, related to the physics of the 858 problem itself, the nature and type of data, the requirements of the solutions. As for the 859 physics of the problem, it is undoubtful that the SSCs degradation processes in practice are 860 most of the times quite complex and dependent on a large number of parameters and 861 mechanisms, which are dynamic and highly non-linear, and not completely known.

But much of the problem comes from the data and the extraction of informative content for the fault detection, diagnostics and prognostics tasks of PHM. Managing and treating the big condition-monitoring data collected by the sensors and comprised of a large variety of heterogeneous signals is not an easy task and the data are often anomalous, scarce, incomplete and unlabeled. Furthermore, they are collected under changing operational and environmental conditions during the life of the SSC.

868 Surely, for the effectiveness of extracting informative content from data, undoubtedly 869 Deep Learning (DL) has contributed a great leap by incorporating feature engineering in the 870 process of learning of the models, for automatic processing of big and heterogeneous 871 condition monitoring data and extraction of features relevant for the application. Encouraging 872 results have been obtained already in fault detection and diagnostics, whereas Prognostics 873 remains still a challenge for DL.

874 Other of the above challenges are being addressed with sophisticated advancements 875 which need to be, then, effectively deployed in practice. These include: Recurrent Neural 876 Networks for PHM applications, and their transformation into images so as to exploit the 877 powerful methods of image processing (including the novel Convolutional Neural Networks 878 (CNNs), particularly for fault detection and diagnostics; signal reconstruction methods (including Auto-Encoders) of unsupervised and semi-supervised learning for fault detection
and diagnostics, and for degradation state prediction, to cope with the frequent practical cases
of unlabeled data; Optimal Transport (OT) methods and unsupervised adaptation techniques
to cope with the problem that the test data distribution may be a different distribution (or
evolve to a different distribution) than that of the training data, with the consequence that the
trained data-learned model may perform poorly on the test data.

885 An issue of particular relevance for the prognostic task of PHM is the proper treatment 886 of the uncertainty in the data and, then, in the models. Several sources of uncertainty exist in 887 practice, as the models are inevitably only representations of the real relationships between 888 input and output, the measured data are inevitably noisy due to measurement errors, and the 889 future operational and environmental profiles of the SSCs are not known. All these 890 uncertainties affect the predictions of the future degradation and failure of the SSCs. With 891 respect to the uncertainty issue in PHM, frameworks are being developed for a probabilistic 892 treatment of the RUL of SSCs: given the potentially costly and catastrophic consequences 893 associated with the decisions that are made based on the PHM outcomes, it is obsolutely 894 necessary to provide also estimates of the uncertainty alongside the predictions. Fore 895 example, frameworks are being developed by Bayesian neural networks and deep gaussian 896 processes.

897 An issue which is arising with the data-driven models and algorithms used for PHM is 898 that they lack interpretability, which reduces trust in their use particularly for safety-critical 899 applications. This leads to the need to find ways for improving transparency an 900 interpretability for a clearer understanding of what the model predicts and how, and finally for 901 building trust on its use. Methods for injecting physical information in learning models, post-902 hoc sensitivity approaches and visualization techniques are being studied to provide 903 interpretability from different perspectives, including explaining the learned input-output 904 relation representations, explaining the individual model outputs, explaining the way the 905 output is produced by the model.

906 Strong concerns are also arising with respect to the security of PHM models for real 907 applications, in particular for safety-critical ones. PHM is increasingly used to support 908 maintenance decision-making processes in various high-value/high-risk industries, where the 909 wrong decision may result in serious consequences. The methods and models used perform 910 exchange and elaboration of data, and must then be secure to reject training data with negative 911 impacts on the results of decision-making.

912

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