Physics Enhanced Machine Learning for Monitoring and Twinning

MARCUS HAYWOOD-ALEXANDER, KIRAN BACSA, WEI LIU, ZHILU LAI and ELANI CHATZI

ABSTRACT

To ensure a resource-efficient and resilient operation of engineered systems, it is imperative to understand their performance as-is; a task which can be effectuated through Structural Health Monitoring (SHM). When considering higher levels of the SHM hierarchy, purely data-driven methods are found to be lacking. For higher-level SHM tasks, such as prognosis, or for furnishing a digital twin of a monitored structure, it is necessary to integrate the knowledge stemming from physics-based representations, relying on the underlying dynamics and mechanics principles. This paper discusses implementation of such a *physics-enhanced* approach to SHM.

INTRODUCTION

The rise in computing power and data availability has favoured the assimilation of Machine Learning (ML) and Deep Learning (DL) techniques within engineering applications [1, 2]. While this surge tends to motivate purely data-driven applications, such methods suffer shortcomings when challenged with tasks that require generalisation and/or extrapolation potential. This is often the case within the context of Structural Heath Monitoring, where further to the task of diagnosis, it is essential to execute tasks related to prognosis. Traditionally, prognostic tasks have relied on *white-box* engineering models, often configured a priori, for forecasting structural performance or inferring response in locations where measurements are not available; the latter is known as the virtual sensing task [3]. To exploit data availability, the so-called hybrid - or *grey-box* - approach to modelling has emerged, where data is fused with *physics-based* engineering models, in order to refine predictive potential. While hybrid models need not rely on ML/DL tools, recent years have seen the surge of *physics-enhanced* ML (PEML) schemes into the SHM domain.

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Perhaps one of the most typical examples of a hybrid approach to monitoring of dynamical systems is delivered in Bayesian filter estimators, which couple a system model (typically in state-space form, but often inferred from numerical (e.g. finite element models), with sparse and noisy monitoring data. Such Bayesian filters can be used for estimation tasks of different complexity, including pure response (state) estimation, joint or dual state-parameter estimation, input-state estimation, and even joint state-parameter-input identification [4]. Bayesian filters draw their potency from their capacity to deal with uncertainties stemming from modelling errors, disturbances, lacking information on the model and its loads (inputs), and noise corruption. However, they are limited by the requirement for a model structure, which should be representative of the system's dynamics.

In relaxing such an assumption, it would be important to deliver system representations that can more flexibly account for our lack of knowledge of the underlying physics. PEML methods fulfil this goal by leveraging known physics to enhance *black-box* ML-based predictors, improving their generalisability, learning efficiency, and interpretability [5]. Inspired by the categorisation put forth in the recent work of Faroughi *et al.* [5], this paper presents three styles of physics-embedding methods across different areas of the spectrum illustrated in Figure 1; physics-guided methods, physics-informed methods, and physics-encoded learners.

- *Physics-guided* methods assume exhaustive physical models, enforcing stricter constraints on the embedded physics. The amount of data required depends on the strictness of the imposed physics, albeit data-sparsity concerns are often raised. It is noted that only partial knowledge of the physics can be prescribed, with residual (or model mismatch) terms taken on by learners.

- *Physics-informed* methods strike a balance between purely data-driven and physics-guided approaches. In these methods, the physics is embedded in a less constrained manner, i.e. it is weakly imposed, typically by minimising a loss function, which vanishes when the imposed physics is satisfied.

- Finally, *physics-encoded* learners directly embed physics within the learner's architecture using operators, kernels, or transforms. This results in less restricted modelling (e.g. they may simply impose derivatives), but they are constrained by the requirement to adhere to this construct.

In the next sections, we offer an overview of adoption of these three different classes of PEML schemes within the SHM domain.

THE WHITE BOX CASE - BAYESIAN FILTERING

Prior to overviewing the mentioned PEML classes and their adoption within the SHM and twinning context, we briefly recall the *white-box* case of Bayesian Filtering (BF), featured on the upper left corner of the domain depicted in Figure 1. The equation of motion of a linear time invariant dynamic system can be formulated as [6]:

$$\mathbf{M}\ddot{\mathbf{z}}(t) + \mathbf{D}\dot{\mathbf{z}}(t) + \mathbf{K}\mathbf{z}(t) = \mathbf{S}_i\mathbf{u}(t) \quad (1)$$

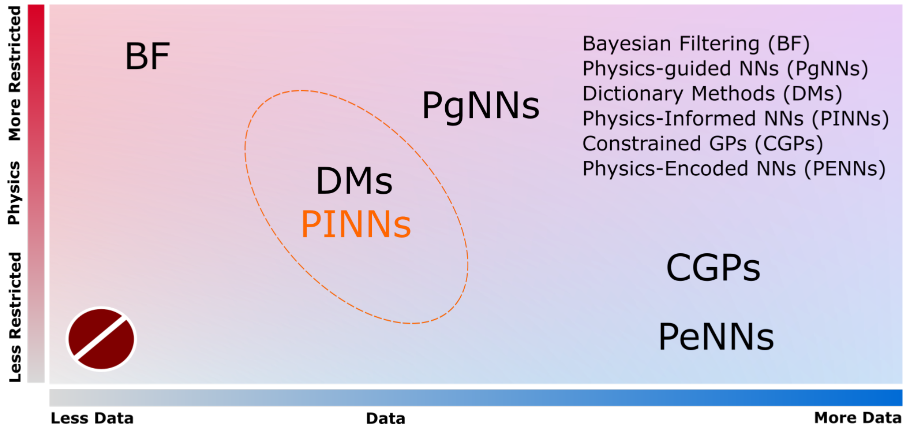

Figure 1. Clustering of *physics-enhanced* ML techniques for monitoring and dynamics.

where $\mathbf{z}(t) \in \mathbb{R}^{n_{dof}}$ is the vector of displacements, often linked to the Degrees of Freedom (DOFs) of a numerical system model, $\mathbf{M} \in \mathbb{R}^{n_{dof} \times n_{dof}}$, $\mathbf{D} \in \mathbb{R}^{n_{dof} \times n_{dof}}$ and $\mathbf{K} \in \mathbb{R}^{n_{dof} \times n_{dof}}$ denote the mass, damping and stiffness matrices respectively; $\mathbf{u}(t) \in \mathbb{R}^{n_i}$ (with n_i representing the number of loads) is the input vector and $\mathbf{S}_i \in \mathbb{R}^{n_{dof} \times n_i}$ is a Boolean input shape matrix for load assignment. As an optional step, a Reduced Order Model (ROM) can be adopted, often derived via superposition of modal contributions $\mathbf{z}(t) \approx \mathbf{\Psi}\mathbf{p}(t)$, where $\mathbf{\Psi} \in \mathbb{R}^{n_{dof} \times n_r}$ is the reduction basis and $\mathbf{p} \in \mathbb{R}^{n_r}$ is the vector of the generalised coordinates of the system, with n_r denoting the reduced system dimension. This allows to rewrite Equation 1 as:

$$\mathbf{M}_r\ddot{\mathbf{p}}(t) + \mathbf{D}_r\dot{\mathbf{p}}(t) + \mathbf{K}_r\mathbf{p}(t) = \mathbf{S}_r\mathbf{u}(t) \tag{2}$$

where the mass, damping, stiffness and input shape matrices of the reduced system are obtained as $\mathbf{M}_r = \mathbf{\Psi}^T\mathbf{M}\mathbf{\Psi}$, $\mathbf{D}_r = \mathbf{\Psi}^T\mathbf{D}\mathbf{\Psi}$, $\mathbf{K}_r = \mathbf{\Psi}^T\mathbf{K}\mathbf{\Psi}$ and $\mathbf{S}_r = \mathbf{\Psi}^T\mathbf{S}_i$. The system can be eventually brought into a combined deterministic-stochastic state-space model, which forms the basis of application of Bayesian filtering schemes [3]:

$$\begin{cases} \mathbf{x}_k = \mathbf{A}_d\mathbf{x}_{k-1} + \mathbf{B}_d\mathbf{u}_{k-1} + \mathbf{w}_{k-1} \\ \mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{G}\mathbf{u}_k + \mathbf{v}_k. \end{cases} \tag{3}$$

where the state vector $\mathbf{x}_k = \begin{bmatrix} \mathbf{p}_k{}^T & \dot{\mathbf{p}}_k^T \end{bmatrix}^T \in \mathbb{R}^{2n_r}$ reflects a random variable following a Gaussian distribution with mean $\hat{\mathbf{x}}_k \in \mathbb{R}^{2n_r}$ and covariance matrix $\mathbf{P}_k \in \mathbb{R}^{2n_r \times 2n_r}$. Stationary zero-mean uncorrelated white noise sources $\mathbf{w}_k$ and $\mathbf{v}_k$ of respective covariance $\mathbf{Q}_k : \mathbf{w}_k \sim \mathcal{N}(0, \mathbf{Q}_k)$ and $\mathbf{R}_k : \mathbf{v}_k \sim \mathcal{N}(0, \mathbf{R}_k)$ are introduced to account for model uncertainties and measurement noise. Bayesian filters exploit this hybrid formulation to extract an improved posterior estimate of the complete response of the system $\mathbf{x}_k$, i.e. even in unmeasured DOFs, on the basis of a "predict" and "update" procedure. Variants of these filters are formed to operate on linear (Kalman Filter - KF) or nonlinear systems (Extended KF - EKF, Unscented KF - UKF, Particle Filter - PF, etc) for diverse estimation tasks. Moreover, depending on the level of reduction achieved, BF estimators can feasibly operate in real, or near real-time. It becomes, however, obvious that these estimators are constrained by the imposed model form.

THE BLACK BOX CASE - DEEP LEARNING MODELS

At the other end of such a *white-box* (model-based) approach, where the system dynamics is transparent and therefore largely prescribed, lies a *black-box* approach, employing DL schemes to achieve stochastic representations of monitored systems. Linking to the BF structured described previously, Variational Autoencoders (VAE) have been extended with a temporal transition process on the latent space dynamics in order to infer dynamic models from sequential observation data [7]. This approach offers greater flexibility than a strict model-based approach, since VAEs are more apt to learning nonlinear dynamics. The obvious shortcoming is that, typically, the inferred latent space need not be linked to coordinates of physical connotation. This renders such schemes more suitable for inferring dynamical features, and even condition these on operational variables [8], but largely unsuitable for reproducing system response in a virtual sensing context. Following such a scheme, Stochastic Recurrent Networks (STORN) [7] and Deep Markov Models (DMMs) [9], which are further referred to as Dynamic Variational Autoencoders (DVAEs), have been applied for inferring dynamics in a black box context with promising results in speech analysis, music synthesis, edical diagnosis and dynamics [10]. In structural dynamics, in particular, previous work of the authoring team [11] argues that use of the AutoeEncoder (AE) essentially leads in capturing a system's Nonlinear Normal Modes (NNMs), with a better approximation achieved when a VAE is employed [12]. It is reminded that, while potent in delivering compressed representations, these DL methods do not learn interpretable latent spaces.

PHYSICS - ENHANCED ML MODELS

PEML can be leveraged to relax the constraints encountered in a *white-box* approach, while seeding more physics intuition than the *black-box* counterpart. We here adopt the term *physics-enhanced* as an umbrella term encompassing the three main aforementioned categories, which we overview in what follows.

Physics - Guided ML Models

In *physics-guided* Neural Network (PgNN) schemes DL techniques are used to estimate a surrogate mapping between the input (e.g. loads) and target output (e.g. response) datasets, while adhering to prescribed physics, which implies a usually predefined model form. Frequently, this results in the Neural Network (NN) acting as a residual, or transfer function, modeller, determining an estimate of the mapping between the prescribed model and the data. As aforementioned for the case of BFs, when the model is assumed known a priori, the estimation accuracy will suffer in the case of model mismatch. Revach, et al. [13] tackle this challenge by employing a PEML scheme where a NN is embedded within a KF, where partially known process and measurement equations are prescribed, in order to learn the Kalman Gain from data, and feed this in the overall KF flow. Angeli, et al. [14] follow an alternate approach, where a DL framework is trained on data from a generic and computationally intensive multibody model. The reduced model is then fed into an EKF for joint input-state estimation. Similarly, Verhoek et al. [15] additively augment a known approximative state-space (SS) model of a

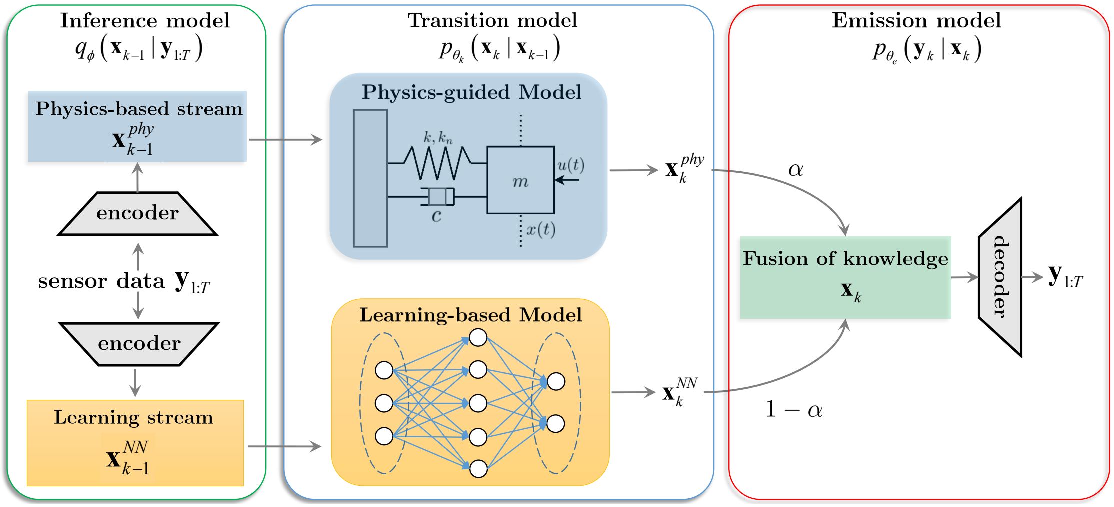

Figure 2. The Physics-guided Deep Markov Model (PgDMM); figure adapted from [16]

nonlinear system with a Sub-Space Encoder Network, which takes on model mismatch. Retaining the additive logic and coupling this to the DMM, our prior work [16] proposed a probabilistic Physics-guided Deep Markov Model (PgDMM) for identifying dynamic system models with a physical connotation from measurement data. The framework, which is illustrated in Figure 2, combines physics-based state-space models with Deep Markov Models, resulting in a hybrid modelling approach. The physics-based models need not fully reflect the state dynamics (e.g. linearised models can be adopted). However, the inductive bias of the partially known physics yields a structured nature of the transition and emission functions in the PgDMM, which leads to a more physically interpretable latent space. This is shown to generalise the predictive capabilities of deep learning-based models on both simulated and experimental use cases.

Physics - Informed ML Models

Physics Informed Neural networks (PINNs) have become a primary instance of *physics-informed* ML-based models. PINNs typically prescribe the model in terms of derivatives in the loss function [17] by exploiting automatic differentiation. The PINN offers a flexible formulation, which can shift weight between physics and data requirements by appropriate assignment of hyperparameters. On the physics side, the objective is often to satisfy prescribed model equations (e.g. governing differential equation). Dictionary methods follow a similar logic [18], attempting to discover a model definition on the basis of a predefined dictionary of possible model solutions. As these methods often impose soft conditions, mismatch between the model and available data is tolerated, rendering these schemes suitable for handling noisy observations. PINNs offer the advantage of incorporating multiple elements within their loss function, including embedment of boundary conditions, complex geometries, and governing equations. PINNs have been demonstrated for simultaneous input-state-parameter estimation tasks in the works of Yuan, et al. [19] and Moradi, et al. [20], on the problem of a monitored vibrating beam. Further works, explore use of PINNS for parameter identification of nonlinear dynamic systems [21] and damage detection [22].

Physics - Encoded ML Models

Physics-encoded schemes embed the physical constraints directly within the estimating operator [23]. An advantage of physics encoded schemes, such as Physics-enhanced NNs (PeNNs), is their extension from instance learning (a frequently commented flaw of PINNs), to more generalised models. An example of *physics-encoded* learners is found in Gaussian processes (GPs). There are two main approaches to embed physical knowledge into GPs, namely i) an appropriate selection of the mean function [24] and ii) via kernel design, where each kernel embeds a different belief as to which family of functions describes the model solution [25, 26]. Such an encoding is further feasible in DL architectures, as yielded in Neural Ordinary Differential Equations (NODEs) [27]. NODEs offer a flexible and expressive modelling framework capturing intricate temporal dependencies and nonlinear dynamics. They inherently accommodate irregularly sampled or sparse data as the ODE solver can handle time interpolation. Moreover, they can leverage established physical laws or prior knowledge by integrating these into the ODE function, thereby augmenting model interpretability and generalisation. In prior work, we enhance standard NODEs by incorporating physical knowledge into the model architecture, to improve structural identification of monitored systems [28]. This so-called physics-informed NODE reflects a versatile framework for discrepancy modelling, with transparentisation of the trained neural network further achieved by coupled implementation of a sparse identification scheme operated on the derived NN. An alternative approach to physics encoding is imposition of constraints according to the Hamiltonian formalism. Greydanus et al. [29] enforce a symmetric gradient on a NN trained to predict the dynamics of a conservative system. Saedmunsson et al. [30] coupled this scheme with the NODE, yielding the so-called Symplectic NODEs. In recent work [31], we extend this reasoning to stochastic learning, where a symplectic encoder, employed within a DMM, learns an energy-preserving latent representation of the system, opening up new directions for use of PeNNs for monitoring of dynamical systems.

DISCUSSION AND CONCLUDING REMARKS

We overview and propose different classes of PEML schemes for achieving tasks of different intricacy within the context of monitoring and twinning. The flexibility of the ML-based learners allows to more flexibly account for model mismatch or to even discover the system's solution and underlying equations, while admitting data of various formats (e.g. images, or video frames) and noise contamination levels. More importantly, the physics bias ensures recovery of latent spaces that have a physical connotation and are, therefore, interpretable [16]. We argue that in all cases physics can be leveraged to serve as an invaluable inductive bias to facilitates the task at hand.

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