Towards the True Hybrid

Physics-informed Trainable Models for Prognostics and Health Management

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KBR Inc., NASA Ames Research Center

RISE Seminar, Virtual, August 2022

Diagnostics & Prognostics Group

Where we are within NASA Ames Research Center

NASA Ames Research Center, Mountain View, CA

↓

Intelligent Systems Division (TI)

↓

Autonomous Systems & Robotics

- Advanced Control & Evolvable Systems
- Deployable Automation Technologies
- Intelligent Robotics
- Planning & Scheduling

Collaborative & Assistant Systems

- Data Repository Systems
- Decision Support Systems
- Enterprise Information Management
- Ground & Flight Data Systems
- Information Integration

Discovery and Systems & Health

- Data Sciences
- Diagnostics & Prognostics
- ISHM Technology Insertion
- Applied Physics
- Quantum Computing
- Computational Materials

Robust Software Engineering

- Core Avionics & Software Technologies
- System Thinking, Architecture & Collaboration
- Models & Algorithms for Reliable Software
- Assured Autonomy

Diagnostics & Prognostics Group

- **Group Leadership**: Chris Teubert (Lead), Wendy Okolo (Deputy)
- **SHARP Lab Manager**: George Gorospe
- **Researchers**: Edward Balaban, Portia Banerjee, Matteo Corbetta, Rajeev Ghimire, Katelyn Jarvis, Chetan Kulkarni, Molly O'Connor, David Nishikawa, Adam Sweet, Jason Watkins

Group's Areas of Contribution

NASA Space Missions & Ground Support	NASA Aeronautics & Air Traffic Management	Growing a robust PHM Community: join PCoE!

Diagnostics & Prognostics Group

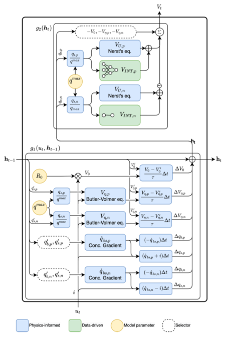
Research Areas

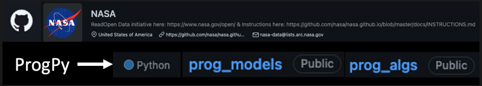
- Diagnostics & prognostics: physics-based and data-driven models and algorithms
- Safety metrics for low-altitude airspace quantification
- Uncertainty quantification and propagation
- Resource-constrained prognostics
- Test-bed development and automated testing for prognostics
- Software architecture for prognostics

Diagnostics & Prognostics Group

Current Works

- System-Wide Safety Project
- Data-Reasoning Fabric
- Distributed Spacecraft Autonomy
- Autonomous Spacecraft Operations
- Software for Prognostic Models and Algorithms: Python's Package *ProgPy*
- Physics-Informed Machine Learning for Next-Gen Electric Aircraft Powertrain





Acknowledgements

Thank to all people who contributed (more or less heavily) to the physics-informed machine learning material in here. In particular:

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- University of Central Florida: Renato G. Do Nascimento, Felipe Viana
- University of Granada (Spain): Manuel Chiachio, Juan Chiachio, Juan Fernandez
- All the authors of the papers we'll discuss here.

Agenda

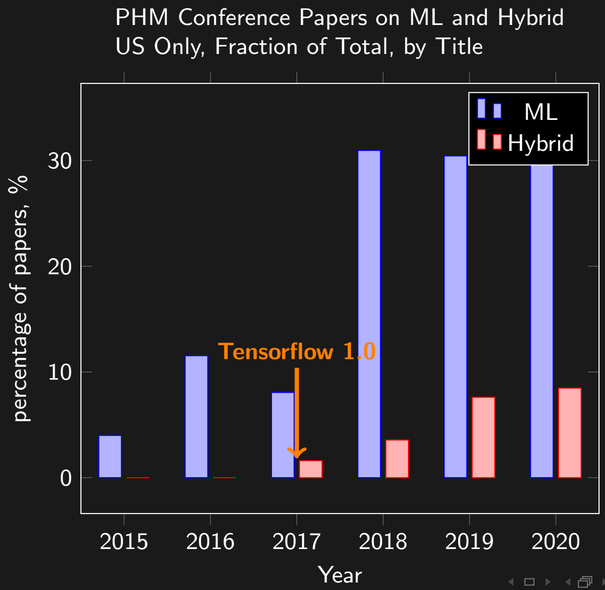
Recent Increase in Machine Learning Papers for PHM

Why to Leverage Physics-Informed Learning in PHM

Overview of Promising Research in Physics-Informed Machine Learning
- Physics-Constrained Gaussian Processes
- Physics-Informed Neural Networks
  - Network-Embedded Models

Concluding Remarks

Recent Increase in Machine Learning Papers for PHM



Why to Leverage Physics-Informed Learning in PHM

Why Machine Learning in the First Place

Great achievements of ML in many scientific areas

Noteworthy, not-so-new papers:

- *AI system for breast cancer screening, Nature, Jan 2020*
- *Generating "Art" by Learning About Styles and Deviating from Style Norms. ICCC, June 2017*
- *DeepFace: Closing the Gap to Human-Level Performance in Face Verification, CCVPR, June 2014*

Why to Leverage Physics-Informed Learning in PHM

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Specificity of Existing Models

- Text-book-like models often applies to simple cases; real systems are a different story
- Flexibility of machine learning and its "black-box" behavior is very appealing. Learn the tool and not the field (Generalist better than specialist, *... is it?*)
- Nowadays, collecting data is cheaper than developing a model

Why to Leverage Physics-Informed Learning in PHM

Potential Advantages of Physics-Informed ML

"Data is the new oil"

The Economist, cover story, May 6th, 2017.

Why to Leverage Physics-Informed Learning in PHM

Potential Advantages of Physics-Informed ML

"Data is the new oil"

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"Data is the new *snake*-oil; because when we'll have better *models*, we'll need *less data*."

Stuart Russel, UAI Conference, Monterey, CA, August 2018

Why to Leverage Physics-Informed Learning in PHM

Potential Advantages of Physics-Informed ML

Why can be worth it

- Ignore the (partial) knowledge we have doesn't seem very clever
- Restrict the search in the parameter space can save data and time
- Improve generalization and extrapolation to unseen input
- Improve *interpretability*

Well-Known Drawbacks of Pure Data-Driven Methods

- Need of data we (typically) do not have in PHM; either data is scarce or we don't have the right data (infrequent failures that have serious consequences)
- Poor interpretability due to: large number of parameters, lack of physical meaning
- Validation and Generalization are hard when: cannot record or don't know we need to record external forcing and other confounding influences, and model needs to extrapolate outside the training domain (i.e., every failure prognosis case!)

Why to Leverage Physics-Informed Learning in PHM

Questions?

Overview of Promising Research in Physics-Informed Machine Learning

Physics-Constrained Gaussian Processes

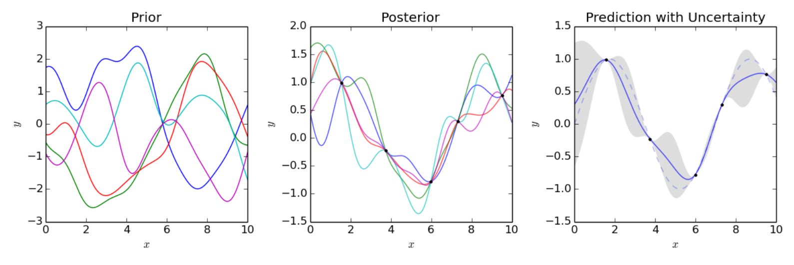
Thanks to Stefan Schuet (NASA Ames) for most of the work here.

Physics-Constrained Gaussian Processes

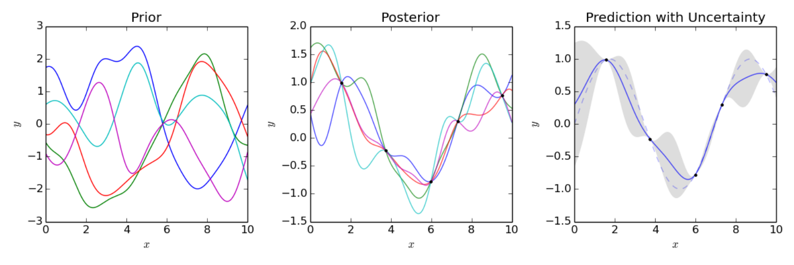
Gaussian Processes (from *Rasmussen & Williams, 2006*)

A Gaussian Process (GP) is a collection of random variables, any finite number of which has a joint Gaussian distribution.

Think of sampling functions from a function space instead of sampling variables:
(image from Wikipedia: wiki/Gaussian_process)



Physics-Constrained Gaussian Processes



$$\boldsymbol{y} \sim \mathcal{GP}\left(m(\boldsymbol{x}), \Sigma_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{x}')\right)$$

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{y}_* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} m(\boldsymbol{x}) \\ m(\boldsymbol{x}_*) \end{bmatrix}, \begin{bmatrix} k_{\boldsymbol{\theta},\boldsymbol{xx}} + \sigma_n^2 I & k_{\boldsymbol{\theta},\boldsymbol{xx}_*} \\ k_{\boldsymbol{\theta},\boldsymbol{xx}_*}^\top & k_{\boldsymbol{\theta},\boldsymbol{x}_*\boldsymbol{x}_*} \end{bmatrix} \right)$$

$$\boldsymbol{y}_* | \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta} \sim \mathcal{GP}\left(\tilde{\mu},\ \tilde{\Sigma}\right)$$

Physics-Constrained Gaussian Processes

Use of Physics-Informed GPs

Surrogate models of complex physical phenomena

- Trainable with few data-points
- Fast to run w.r.t. FEM, CFD,
- Improve extrapolation

Physics-Constrained Gaussian Processes

From GPs to Physics-Informed GPs

Function we want to approximate (unknown) $f(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^{n \times 1}$

We also know from the physics that $\mathcal{L}_{\boldsymbol{x}} f(\boldsymbol{x}) = 0$

Physics-Constrained Gaussian Processes

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Physics-Constrained Gaussian Processes

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Vector $[\hat{f}(\boldsymbol{x}), \mathcal{L}_{\boldsymbol{x}} f(\boldsymbol{x})]^\top$ is also a $\mathcal{GP}$

- $\hat{f}$ is a $\mathcal{GP}$ (holds linear properties)
- Derivatives are linear operations
- The problem is to find the derivative of the $\mathcal{GP}$ mean function and covariance matrix

Physics-Constrained Gaussian Processes

Example: Heat Equation

Additive manufacturing: learn a surrogate model of the manufacturing process to map material properties as function of process parameters, constraining the surrogate model with known physics

Physics-Constrained Gaussian Processes

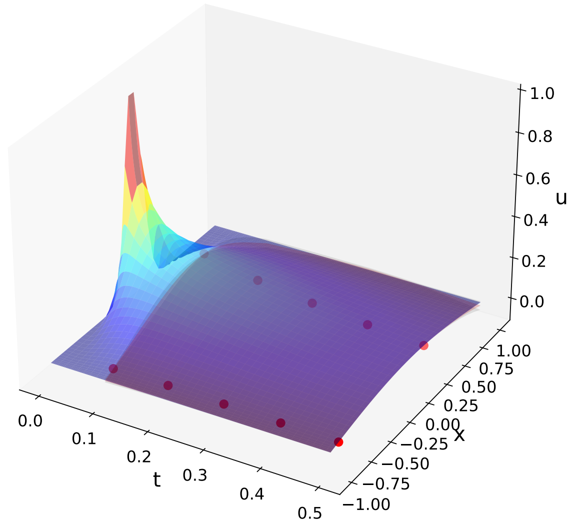
Example: Heat Equation (simplest case)

$$f(x,0) = \delta_{x,0}$$

$$\mathcal{L}_{\boldsymbol{x}} f(\boldsymbol{x}) = \frac{\partial f(x,t)}{\partial t} - \alpha \frac{\partial^2 f(x,t)}{\partial x^2} = 0$$

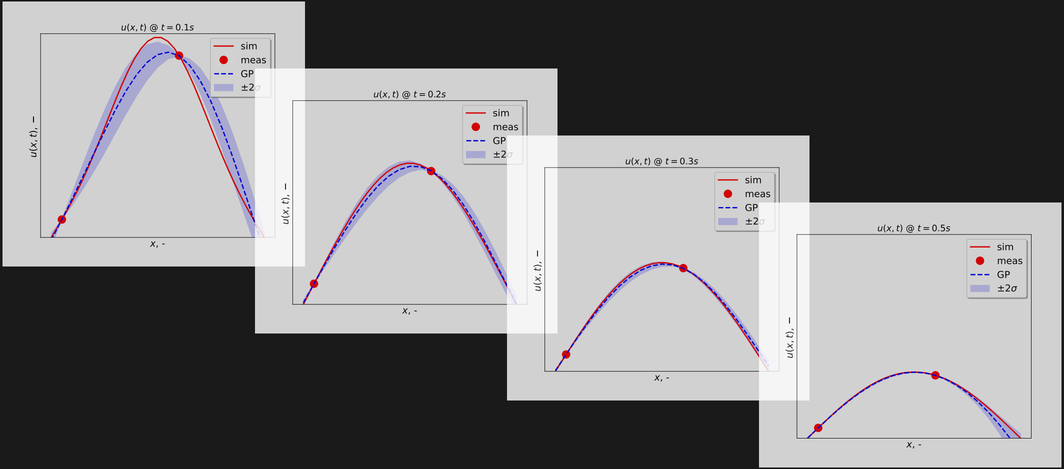
$$\begin{bmatrix} \hat{f}(x,t) \\ \hat{f}_t - \alpha \hat{f}_{xx} \end{bmatrix} \sim \mathcal{GP}(\tilde{m}, \tilde{\Sigma})$$

Simulated with Matlab (analytical solution)



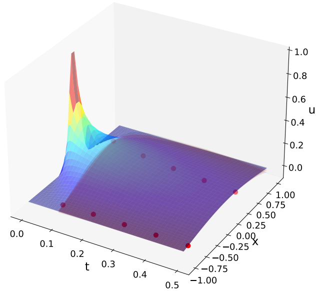
Physics-Constrained Gaussian Processes

Heat Equation



Physics-Constrained Gaussian Processes

Problems



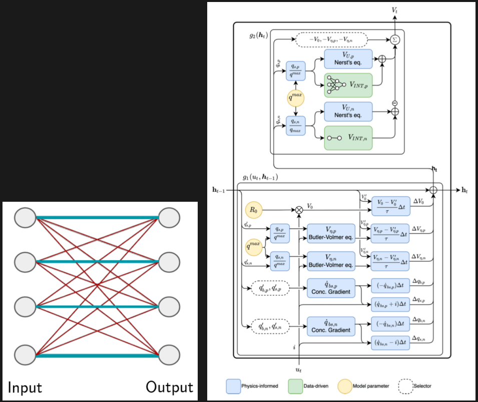
1. Covariance matrices are big and built upon symbolic calculus. It's time consuming and creates hyper-parameter optimization issues.
2. Physical processes are characterized by varying lengthscales in time, space, or both (that's why we didn't fit the beginning!). In this example, a kernel function with a single lengthscale parameter cannot fit well the very sharp heat drop (start) and the slow heat diffusion (later) in the process. Need of a *non-stationary* covariance function for that.
3. Solution to problem #2 makes the solution to problem #1 more challenging

Physics-Constrained Gaussian Processes

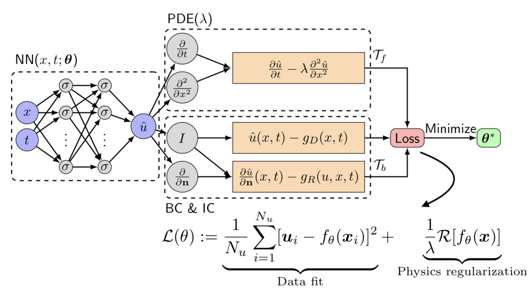
References and Q&A

1. http://www.gaussianprocess.org/gpml/ (Rasmussen & Williams)
2. Rasmussen et al. Gaussian processes in machine learning, 2003
3. Constantinescu et al. Physics-based covariance models for Gaussian processes with multiple outputs. *International Journal for Uncertainty Quantification* 3;1, 2013
4. Jidling et al., Linearly constrained Gaussian processes, 2017
5. Lange et al. Algorithmic linearly constrained Gaussian processes, 2018.

Physics-Informed Neural Networks



(a) Zaheer et al. Deep Sets, 2017; Viana, Nascimento, 2021



(b) Prof. Paris Perdikaris, AAAI-MLPS 2020

Figure: Implicit (a) and Explicit (b) constraints in neural networks.

Physics-Informed Neural Networks

Implicit Constraints:

- **Constrained-Connection Networks**: Build a trainable model with ad-hoc connections and equations, so that parameters are driven by physics.
- **Hybrid – Network-Embedded Models**: insert neural networks (e.g., MLPs) within a bigger model to learn unknown relationships, uncertainty parameters, etc.

Explicit Constraints:

- **Physics-driven loss function**: physics is explicity imposed in the output by adds-on to the loss function; if the solution does not satisfy physical constraints, the loss goes up

Battery Discharge and Aging Prediction with Implicit PINN – Tensorflow & PyTorch

Thanks to:
Felipe Viana (UCF),
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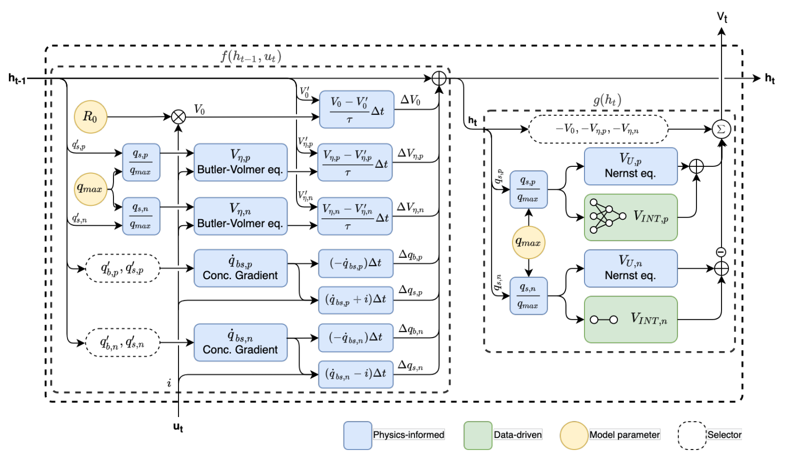
Stefan Schuet (NASA Ames),
Chetan Kulkarni (KBR, NASA Ames)

Network-Embedded Models

Battery Discharge and Aging Prediction with Implicit PINN – Tensorflow

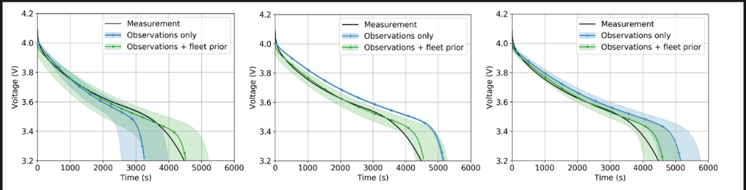


Predict voltage curve during operation and battery aging

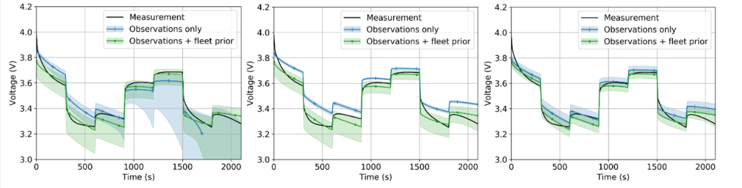
- Parameters R_0 and q_{max} estimated after each discharge
- Interval voltages $V_{INT,\cdot}$ approximated using MLPs

Network-Embedded Models

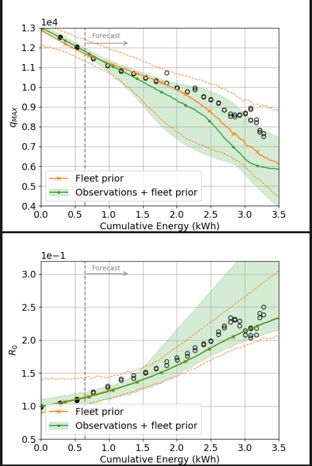
Battery Discharge and Aging Prediction with Implicit PINN – Tensorflow



(a) Reference discharge.



(b) Random-loading discharge.



Network-Embedded Models

Problems

- Careful tuning of initial values is still a thing
- Optimizers don't know physical limits of parameters $\rightarrow$ huge or small numbers trying to compensate for model errors. When you limit them, the optimization can get stuck in local minima.
- Uncertainty estimate possible with *Variational layers*, but deep learning frameworks are still not perfect at handling those.

Physics-Informed Neural Networks

References and Q&A

1. Dourado et al. Physics-informed neural networks for missing physics estimation in cumulative damage models: a case study in corrosion fatigue. *Journal of Computing and Information Science in Engineering*, 2020
2. Nascimento et al. Fleet prognosis with physics-informed recurrent neural networks, 2019
3. Fricke et al. Quadcopter Soft Vertical Landing Control with Hybrid Physics-informed Machine Learning, *AIAA SCITech Forum*, 2021
4. Zaheer et al., Deep Sets, 2017
5. Gens et al, Deep symmetry networks, 2014

Other Works

There's been MUCH MORE on these topics that I haven't covered:

1. Kaiser et al., Data-driven discovery of Koopman eigenfunctions for control. *Proceedings of the Royal Society A*, 2018
2. Lu et al. Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. *Nature Machine Intelligence*, 2021
3. Chen et al. Neural Ordinary Differential Equations. *NIPS*, 2018.
4. Cranmer et al. Lagrangian Neural Networks. *NIPS*, 2020.
5. ...

Concluding Remarks

Remembering the Why

- Learning degradation leveraging data-driven tools when amount of data is scarce, and/or when there's not enough information to build a model, but, having 'some' knowledge is common.
- System identification and system-level prognostics: learning complex system dynamics as faults / degradation evolve in individual components or sub-systems. This requires powerful learning algorithms, but we need to understand how to systematically limit over-fitting (and under-fitting) to make them work properly.

Thank you

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