From Physics-based Models to Predictive Digital Twins via Interpretable Machine Learning

Michael Kapteyn*, Prof. Karen Willcox
INFORMS 2020 | November 13, 2020
1 Motivation
Predictive digital twins to inform critical decision-making

2 Methodology
Interpretable data-driven adaptation of physics-based models

3 Results
Enabling a self-aware UAV: progress and outlook
An aircraft that can sense changes in its own internal state, and adapt accordingly.

Prior work has shown that this provides [Kordonow 2011, Singh 2017]
- Increased survivability
- Increased utilization
Motivation: Enabling a self-aware aircraft

We create a digital twin that adapts to the evolving structural health of the UAV, providing near real-time capability predictions to enable dynamic decision-making.
Toward predictive, reliable, explainable digital twins

**Physics-based models**

- Ubiquitous throughout engineering
- Simulate new previously unseen scenarios
- Obey laws of physics with quantifiable uncertainty
- Parameters represent real-world quantities

predictive digital twin

interpretable machine learning

physics-based models
Toward **predictive, reliable, explainable** digital twins

### Physics-based models
- Ubiquitous throughout engineering
- Simulate new previously unseen scenarios
- Obey laws of physics with quantifiable uncertainty
- Parameters represent real-world quantities

### Data-driven models
- Leverage the explosion in data availability
- Enable asset-specific decision-making
  - Typically “black-box”
  - Difficult or impossible to understand and explain
  - Generalization requires representative training data

---

Physics-based models

predictive digital twin

interpretable machine learning
Toward **predictive, reliable, explainable** digital twins

**Physics-based models**
- Ubiquitous throughout engineering
- Simulate new previously unseen scenarios
- Obey laws of physics with quantifiable uncertainty
- Parameters represent real-world quantities

**Data-driven models**
- Leverage the explosion in data availability
- Enable asset-specific decision-making
  - Typically “black-box”
  - Difficult or impossible to understand and explain
  - Generalization requires representative training data

**Our approach:**
Interpretable machine learning models trained on physics-based models
Predictive Digital Twin: Physics-based models meet data-driven learning

**Offline:**
- Construct library of physics-based models representing different asset states
- Use model library to train a classifier that predicts asset state based on sensor data

**Online:**
- Sensor data
- Current digital twin
- Analysis, Prediction, Optimization
- Updated digital twin
Physics-based model library
Given: a library of models for various UAV damage states
• Covers representative damage states
• Enables assimilation of sensor measurements (strain)
• Enables estimation of flight capability (stress, failure criteria)

How to choose an appropriate model from the library?
→ Informed by online sensor data

• Which sensors to install?
• Which sensors to query?
• Decision boundaries?
• Reliability + robustness

From physics-based model library to predictive digital twin

Increasing effective damage (reduction in stiffness)

Damage region

Details: [Kapteyn et al., IJNME 2020]
Interpretable machine learning
1. Use **predictive models** to **generate training data**

Training data: \((X, y)\)

- **Features,** \(X\): Model predictions of strain at strain gauge locations, corrupted with random noise
- **Labels,** \(y\): Location and severity of damage (2 locations, 5 severity levels = 25 possible states)
Onboard sensors inform which model is used in the digital twin

1. Use **predictive models** to generate training data
2. Use **machine learning** to train an **interpretable, explainable reactive model**

Forward (predictive) model

Inverse (reactive) model

Training data: \((X, y)\)

Features, \(X\): Model predictions of strain at strain gauge locations, corrupted with random noise

Labels, \(y\): Location and severity of damage (2 locations, 5 severity levels = 25 possible states)
Interpretable machine learning via optimal classification trees

**Goal:** Find a binary tree, $T$, that partitions the space of possible sensor measurements, and assigns to each partition the model that best explains the measurements

$$T : x \rightarrow y$$

*Optimal Classification Trees* [Bertsimas, 2019] uses mixed-integer optimization techniques to find a partition in the form of an optimal binary tree, $T$:

$$\min_T R(T) + \alpha |T|$$

- Globally optimal
- Scalable
- Naturally extends to hyperplane splits
Optimal classification trees in practice: damage in region 1
Optimal classification trees in practice: damage in region 1

Training Data

Classification Tree for Region 1

Sensor locations

Region 1

Region 2
Optimal classification trees in practice: damage in region 2

Training Data

Classification Tree for Region 2

Sensor locations
Onboard sensors inform which model is used in the digital twin

Accuracy depends on:
1. Depth of the tree
2. Split complexity (maximum number of sensors in each split)
Onboard sensors inform which model is used in the digital twin

Accuracy depends on:
1. Depth of the tree
2. Split complexity (maximum number of sensors in each split)
3. Sensor placement

Physics-based model allows us to simulate many candidate sensors
Optimal classification trees scale to allow many input features
Accuracy depends on:
1. Depth of the tree
2. Split complexity (maximum number of sensors in each split)
3. Sensor placement

Physics-based model allows us to simulate many candidate sensors
Optimal classification trees scale to allow many input features
→ let the optimal classification tree select most informative sensors

Onboard sensors inform which model is used in the digital twin

Candidate sensor locations

= optimal sensor locations
Recall our approach: **data-driven adaptation of component-based reduced-order models**

**Offline:**
- Construct library of physics-based models representing different asset states
- Use model library to train a classifier that predicts asset state based on sensor data

**Online:**
- sensor data
- current digital twin
- updated digital twin
- Analysis, Prediction, Optimization
Flight of the UAV

- Aggressive flight path
- Conservative flight path

**Health estimates**

| Less damage | More damage |
|--------------|-------------|
| Sensor 22    | Sensor 22   |
| Sensor 12    | Sensor 22   |
| Sensor 24    | Sensor 22   |

**Strain Measurements**

- Sensor 22
- Sensor 12
- Sensor 24

**Rapid Classification**

- Sensor 22 < 393
- Sensor 22 < 429
- Sensor 22 < 495

- Pristine: 20%
- 40% 60% 80%
Combining physics-based models and interpretable machine learning enables predictive digital twins

Optimal Classification Trees

- Highly interpretable
- Natural framework for sensor selection
- Rapid online classification
- As expressive as standard neural networks

Future Work

- Test with multimodal experimental data
- Strategies for sensor fault detection and robustness
- Flight demonstration
High-consequence decisions require digital twins that are predictive • reliable • explainable

For a project overview and additional references visit https://kiwi.oden.utexas.edu/research/digital-twin

Funding acknowledgements:
• Air Force Office of Scientific Research (AFOSR) Dynamic Data-Driven Application Systems (DDDAS)
• The Boeing Company
• SUTD-MIT International Design Centre