Challenges to Verification and Validation of Data-Driven Models used in Prognostic Health Management of Nuclear Power Plants

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Abstract

• Traditional approaches to V&V for engineering modeling and simulation involve such notions as:
  • geometry,
  • material properties,
  • underlying partial differential equations,
  • boundary conditions, and
  • experimental data
  …many of which are not seamlessly transferrable between first-principle based approaches (e.g., numerical implementations of partial differential equation solutions) and data-driven approaches (e.g., Machine Learning) to modeling and simulation.

• This presentation introduces some of the challenges envisioned regarding how one might establish veracity and validity, predictive capability, and thus credibility for pattern recognition analysis tools in support of plausible objectives pertinent to:
  – Condition Based Maintenance (CBM),
  – Structural Health Monitoring (SHM), and
  – Prognostic Health Management (PHM)

• A hypothesized framework by which V&V may be thought of is presented.
  – Considerations for how software validation testing might be formulated are proposed, in order to demonstrate sufficient quality for effective use in support of prognostic health management of systems, structures, and components (SSC) of a nuclear power plant.

How to approach V&V in Data-Driven modeling for PHM?
Machine Learning and Deep Learning
A Storm is coming… or is it already here?

Leading Companies and Research Institutions in Artificial Intelligence
Ranked by number of world class patents, Competitive Impact>3.5, November 2018

Source: Kai Gramke, Managing Director, EconSight Patent Analytics

<table>
<thead>
<tr>
<th>Company</th>
<th>Patents</th>
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<tr>
<td>Microsoft</td>
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Development of Artificial Intelligence and relevant Sub-Technologies
Active patent families in AI and sub technologies, November 2018

Deep Learning
Deep Learning is a machine learning method that learns by working on multiple layers of data. Each previous layer is used as input for the next layer.

Neural Networks
Neural network is a machine learning model that is inspired by the working of the human brain. It uses observational data to train the model, which then extracts features from the data. A single hidden layer or multiple hidden layers are used.

Machine Learning
Machine learning is a research area of artificial intelligence that applies algorithms to a set of data and learns from that data.
Physics-Based Models

\[ Q = A_2 \sqrt{\frac{2A_1^2(p_2 - p_1)}{\rho(A_2^2 - A_1^2)}} \]

Input 1
Input 2
Input 3
Input 4
Input 5
\ldots
Input n

Output(s)
Data-Based Models: Machine Learning

Input 1 → Output(s)
Input 2 → Output(s)
Input 3 → Output(s)
Input 4 → Output(s)
Input 5 → Output(s)
. → Output(s)
. → Output(s)
Input $n$ → Output(s)
Who’s on First?
ASME vs. ANS vs. IEEE… do we all agree on what V&V is?

- Each organization recognizes the importance of V&V and each has significant influence on the activities of nuclear power plant design, analysis, operations, and maintenance.

<table>
<thead>
<tr>
<th>Term</th>
<th>ASME V&amp;V 10</th>
<th>ANS 10.4</th>
<th>IEEE 1012</th>
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<tbody>
<tr>
<td>Verification</td>
<td>The process of determining that a computational model accurately represents the underlying mathematical model and its solution.</td>
<td>The process of evaluating the products of a software development activity to provide assurance that they meet the requirements defined for them.</td>
<td>The process of evaluating a system or component to determine whether the products of a given development phase satisfy the conditions imposed at the start of that phase.</td>
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<tr>
<td>Validation</td>
<td>The process of determining the degree to which the model is an accurate representation of corresponding physical experiments from the perspective of intended uses of the model.</td>
<td>The process of testing a computer program and evaluating the results to ensure compliance with specified requirements. The demonstration that the verified computer program (and by inference the mathematical model) are an adequate representation of the physical phenomena.</td>
<td>The process of evaluating a system or component during or at the end of the development process to determine whether it satisfies specified requirements. The process of providing evidence that the system, software, or hardware and its associated products satisfy requirements allocated to it at the end of each life cycle activity, solve the right problem (e.g., correctly model physical laws, implement business rules, and use the proper system assumptions), and satisfy intended use and user needs.</td>
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</table>

Notes:
1. The 2018 draft revision to V&V 10 replaces “the real world” with “corresponding physical experiments” relative to the published 2006 guideline.
Pertinence of V&V Workflow pieces to Data-driven Modeling & Simulation

- **Green** – applies
- **Red** – does not apply
  - Preliminary Calculations from Simulation Results informing Experimental Design
- **Yellow** – might apply?
  - Experiment Design
  - Instrumentation Quality Assurance
  - Validation Experiment
  - Code Verification

Much of V&V 10 is Extensible to Data-Driven Modeling, but some portions may not be easily applied
Notional Workflow for Prognostic Health Management

- **How does one **verify** that an anomaly has occurred?**
  - Is the Machine Learning “correct”?

- **How does one **validate** that an anomaly has occurred?**
  - Does some observable physical failure need to occur?

- **What does V&V look like for the stages which follow detection of an anomaly?**
  - **Diagnostics** (e.g., you have cancer)
  - **Prognostics** (e.g., you have ___ years to live)

- **To what extent is mechanistic modeling needed for correct diagnosis?**
  - *i.e.*, are we completely stumped if without?
Example Case for Structural Health Monitoring
Aging of Reactor Vessel Internals

Multiple types of degradation may be present, so when something anomalous is observed…

…which form of degradation is it?

Legend
- Wear
- Stress Corrosion Cracking
- Relaxation
Challenge – Lack of Operating Experience Data

• Most data monitored and stored relate to plant process parameters (e.g., system pressures, temperatures, flows) and not necessarily SSC-specific measurements that would be predictive of component reliability.

• Plants operate in steady state >90% of the time (very low variation data to learn from)

• Components are high reliability with low history of failures. This makes it difficult to perform meaningful failure modes and effects analysis (FMEA), which is required to identify the failure modes upon which to install sensors to monitor.
  – Particularly true of components important to plant safety

• Preventative and corrective maintenance history records often not in a convenient form

Need for organized data sources
Challenge – Uncertainty in Prognostic Modeling

• Epistemic uncertainty in how one actually models/predicts reliability (e.g., is Miner’s rule sufficient?)
• Parametric uncertainty: sparse data makes it difficult to fit models
• There’s some balance between modeling accuracy required and the application:
  – Mission-critical components (e.g., Feed-water pumps, Diesel Generators, pressure boundary) require high confidence in predictions to influence maintenance policy
  – Non-safety components (e.g., balance of plant, power generation-only) may have more flexibility
• Until sufficient OE history developed, it is likely we will use prognostics to “confirm our intuition” (inform) when making maintenance policy decisions, rather than the decisions being based upon the prognostics
  – *Example:* Uber still places drivers in “autonomous” vehicles, and for good reason

How Long until Maintenance Needed?
Challenge – Black Box Nature of Machine Learning Models

• Stochastic nature of model training algorithms
  – Challenge for repeatability

• Trained model architecture and parameters can be highly complex
  – Easily thousands of nodes, arcs, and weights in a neural network
  – Models not easily inspected or interpreted
Chain of Approximations – General

• “All models are wrong, but some are useful”
  – Generally attributed to George Box

Data-driven models offer a different paradigm for approximation of the real world

Picasso’s “Reduced Order” Dog
Chain of Approximations – Applied to Pump

- First principles (i.e., PDEs) differ from data-driven (i.e., Machine Learning) approaches

Software implementations may look quite different depending on the approach
Path from Conceptual Model to Computational Model

- Surrogate modeling may involve another branch to this “tree”

Surrogate (i.e., data-driven version) of Computational Model

from V&V 10

data-driven modeling consideration?
Hierarchical Structure of Mathematical Systems

- Consider pertinence of data-driven “components” of mathematical “assemblies” and “systems”…

Necessity of V&V for data-driven modeling
Mathematics of Anomaly Detection
Considering Support Vector Machine

- Machine Learning algorithms are indeed mathematical models governed by equations
- But they are used to represent physics with some means other than the relevant PDEs associated with the physical phenomena of interest

\[
x: \quad f(x) = x^T \beta + \beta_0 = 0
\]

\[
\max_{\beta, \beta_0, \|\beta\| = 1} M
\]

subject to \( y_i(x_i^T \beta + \beta_0) \geq M, i = 1, ... , N \)

\[
y_i(x_i^T \beta + \beta_0) \geq M(1 - \xi_i)
\]

\[
\min \|\beta\|
\]

subject to \[
\begin{cases}
y_i(x_i^T \beta + \beta_0) \geq 1 - \xi_i & \forall i \\
0 \leq \xi_i \leq \text{constant}
\end{cases}
\]

Hierarchical Modeling may involve not only verification of the PDEs (if applicable) but also the Machine Learning equations used to approximate the PDEs
A Continuum of Needed Information for Diagnostics

Empirical Data

Subject Matter Expertise

Mechanistic Modeling

∫ Available Information

= Meaningful Diagnostics
Motivation for Optimization in “Digital Twinning” for Diagnostics

- **Digital Twin**: An integrated multi-physics, multiscale, probabilistic simulation of an as-built vehicle or system that uses the best available physical models, sensor updates, fleet history, etc., to mirror the life of its corresponding (operating) twin.

- **Inverse Problem**: The class of problems that arise when we have partial information and indirect observations of a system and need to infer (hidden) quantities of interest in the system; can be viewed as a quest for information that is not directly available from observations or measurements.

Optimization is Needed when Outputs ≠ Observation
Uncertainty Quantification and **Propagation** through Workflow

- Some non-negligible error exists at each stage of the serial process of
  1. Anomaly *Detection*
  2. *Diagnostics*
  3. *Prognostics*

- Therefore, to properly characterize the Uncertainty ($U$) for some key result, such as remaining useful life ($RUL$), the uncertainties at each stage must be properly quantified and propagated.

\[
U_{RUL} = \sqrt{U_{Detection}^2 + U_{Diagnostics}^2 + U_{Prognostics}^2}
\]
## Predictive Capability

**Predictive Capability Maturity Matrix (PCMM)**

<table>
<thead>
<tr>
<th>Element of PCMM</th>
<th>Pertinence to Pattern Recognition Analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Representation and geometric fidelity</td>
<td>For a data-driven model, this may pertain to the amount of information available, in terms of the number of relevant variables or the duration over which data has been collected.</td>
</tr>
<tr>
<td>Physics and material model fidelity</td>
<td>This may pertain to the degree to which a predictive model is calibrated/trained to the available data.</td>
</tr>
<tr>
<td>Code verification</td>
<td>This focuses upon the correctness of numerical algorithms relative to a mathematical model, and so may be viewed as the degree to which the training data is represented by the pattern recognition model (with some consideration of over-fitting).</td>
</tr>
<tr>
<td>Solution verification</td>
<td>This deals with numerical solution errors in computed results, such as could be due to method of sampling the available training data, or the architecture of some Machine Learning model (e.g., nodes and layers of an Artificial Neural Network, or number of vectors for a Support Vector Machine).</td>
</tr>
<tr>
<td>Model validation</td>
<td>This focuses on thoroughness and precision of the accuracy assessment of computational results, such as the Root Mean Squared (RMS) error between a predicted and an independently-sampled data set. For example, if 70% of the available data is used for training (and verification), then the remaining 30% of the data might be used for testing (validation).</td>
</tr>
<tr>
<td>Uncertainty Quantification and Sensitivity Analysis</td>
<td>This focuses upon the correctness of Uncertainty Quantification, the propagation of uncertainties, and the thoroughness and precision of a sensitivity analysis to determine the most important contributors to uncertainty in system responses of interest.</td>
</tr>
</tbody>
</table>
**Predictive Capability**

**Convex Hull Method**

- **The convex hull** is the set of points in which, for any given pair of points in the set, all points “linearly in between” are also in the set.
  - Center of mass can be outside the object, but never outside its convex hull.

- Useful for **visualizing** the portions of some $n$-dimensional space the domain of (in)applicability.

- Note locations of minimal sampling…

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**Not Convex**  OR  **Convex**
# Outline for Functional Requirements

<table>
<thead>
<tr>
<th>Category</th>
<th>Thought</th>
</tr>
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<tbody>
<tr>
<td>Data Management</td>
<td>Assemble data to be evaluated in a clean and consistent format.</td>
</tr>
<tr>
<td>Data Visualization</td>
<td>Examine various plots and summary statistics of the data.</td>
</tr>
<tr>
<td>Feature Selection</td>
<td>Identify the parameters to include in the predictive model.</td>
</tr>
<tr>
<td>Split Data into Training/Test Sets</td>
<td>Define the time period (and/or samples) over which training versus testing should be performed</td>
</tr>
<tr>
<td>Model Training</td>
<td>Pass training data through Machine Learning / pattern recognition structure, and adjust model parameters to fit the data</td>
</tr>
<tr>
<td>Model Testing</td>
<td>Compute error with respect to evaluating the trained model against test set.</td>
</tr>
<tr>
<td>Use Predictive Model</td>
<td>Deploy the trained and tested predictive model for desired purpose.</td>
</tr>
<tr>
<td>Diagnostics</td>
<td>Offer explanation to the “why”?</td>
</tr>
<tr>
<td>Prognostics</td>
<td>How long do I have until end of life?</td>
</tr>
</tbody>
</table>

### Pop Quiz
If requirements are formulated from these categories and satisfied, then is the PHM code:

1) Verified, Not Validated
2) Validated, Not Verified
3) Verified and Validated
4) Neither Verified nor Validated
Conclusions

- Data-driven modeling is quickly becoming ubiquitous amongst engineering practitioners in industrial settings, such as nuclear power plants.
- The need for verification and validation is clearly evident for such purposes as:
  - Transitioning from time-based to condition-based maintenance paradigms
  - Maintaining nuclear safety, if monitoring safety-related SSC
  - Increasing the role played by automation/digitization associated with PHM
- Definitions of verification, validation, and predictive capability may not be simply extensible from physics-based modeling & simulation to data-driven modeling.
Westinghouse will remain the first choice for safe, clean and efficient energy solutions.

We enhance our delivery of that vision by living our values:

- Safety & Quality First
- Valuing Ethics, Integrity & Diversity
- Passion for Serving Our Customers Globally
- Dedication to Each Other Through Servant Leadership
- Creating Value for Shareholders, Customers & Employees
- Consistently Delivering Our Commitments