SAND2023-04352C

Sandia National Laboratories

Exceptional service in the national interest

An Introduction to Machine Learning for Mechanics

Sandia National Laboratories

Sharlotte Kramer

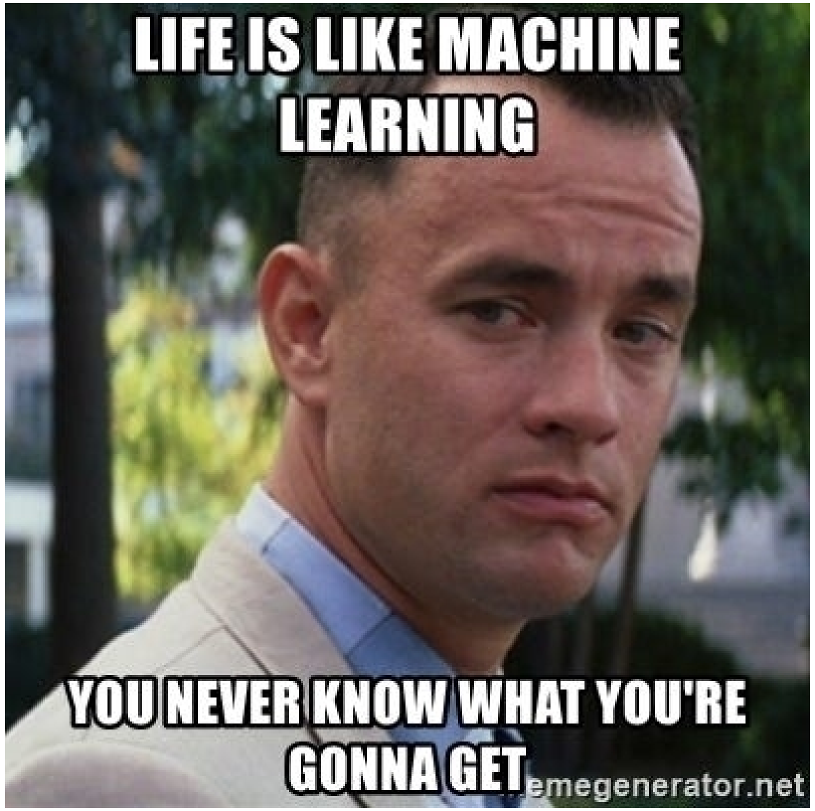
Society of Experimental Mechanics Annual Conference 2023

Orlando, FL

June 5, 2023

Machine Learning (ML) may appear to just be hype and lack rigor and accuracy.

https://analyticsindiamag.com/wp-content/uploads/2017/06/20.jpg



https://medium.com/@krishamehta/10-a-few-useful-things-about-machine-learning-758e2c0149f0

We need some basic understanding of ML to ascertain its value.

The goal of this presentation is to provide a brief introduction to ML for mechanics so you can appreciate and evaluate ML research.

Basic Terms and ML Tasks

Evaluation Approaches

Mechanics Example

Introduction to ML for Mechanics Topics

Basic Terms and ML Tasks

Evaluation Approaches

Mechanics Example

What is Machine Learning?

- Tom Mitchell,
Machine Learning, 1997

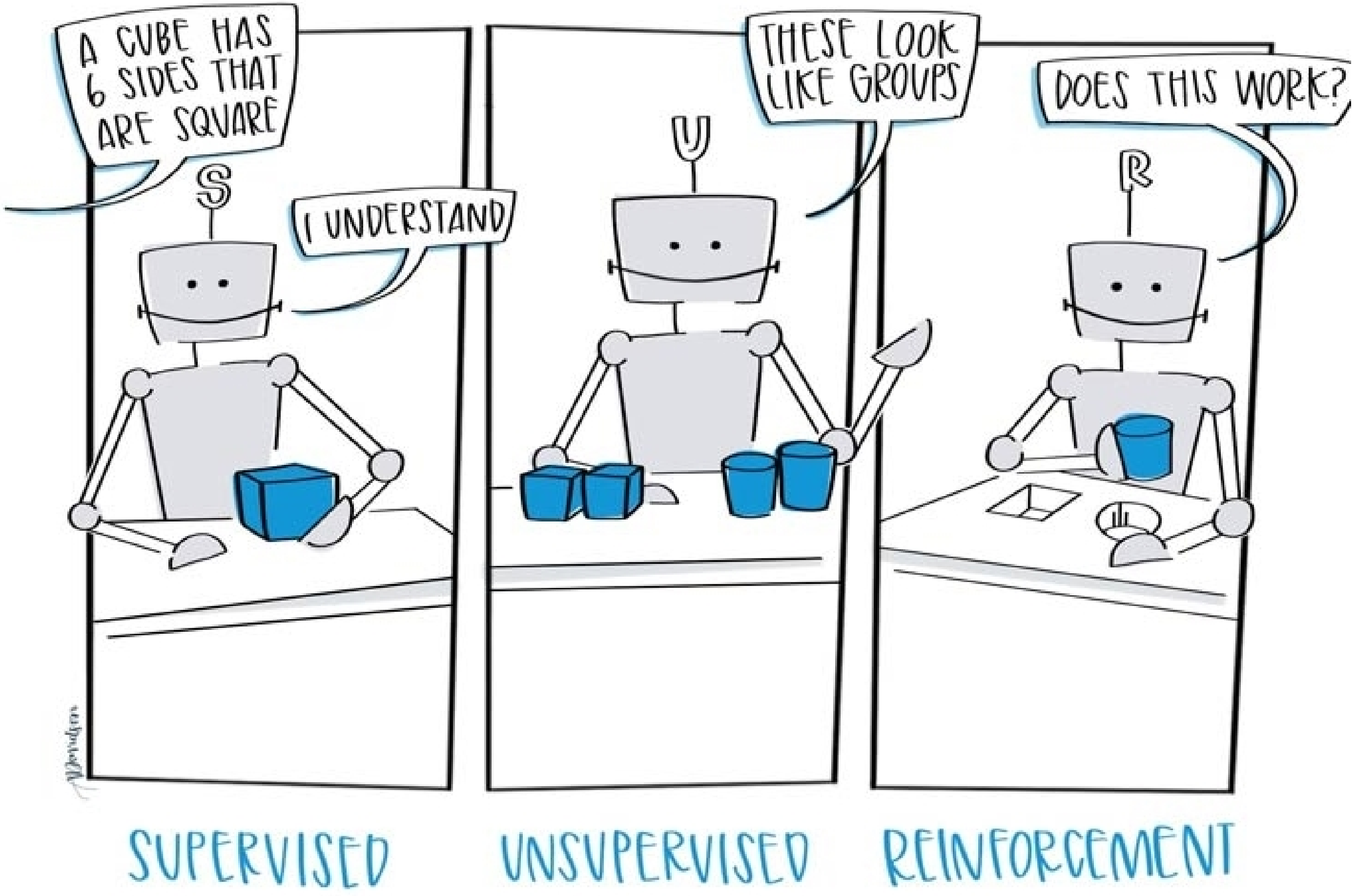
A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

Task (T): Recognizing and classifying defects within SEM images

Performance measure (P): Percent of defects correctly classified

Experience (E): A database of defects with labeled classifications in SEM images

The three main types of ML

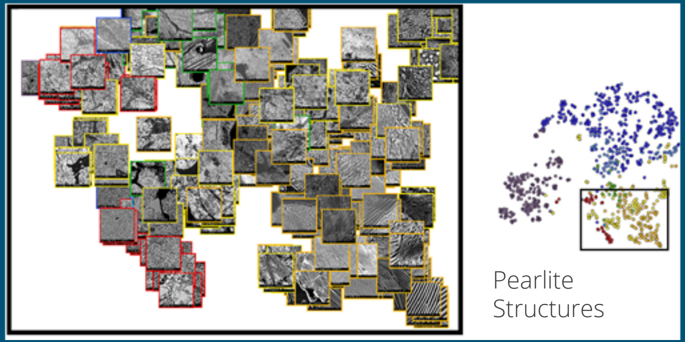


Experience:	Labeled Data	Unlabeled Data	Interaction with Its Environment

Image: https://www.ceralytics.com/3-types-of-machine-learning/

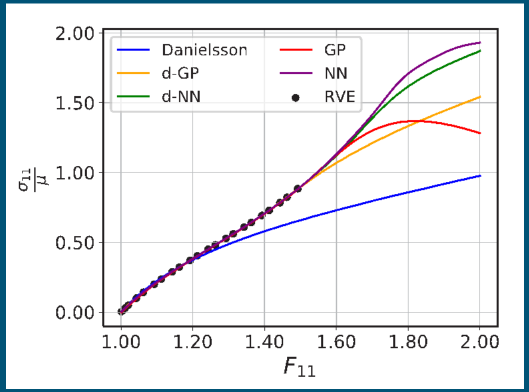
Common ML Tasks

Classification



DeCost, et. al. Acta Materialia 2017

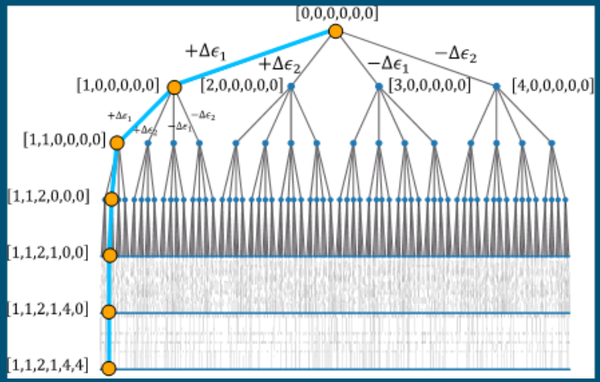
Regression



Polymer
Foam
Mechanics

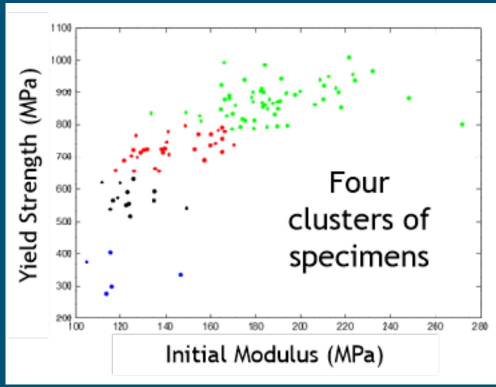
Frankel, et. al. CMAME 2022

Decision-Making



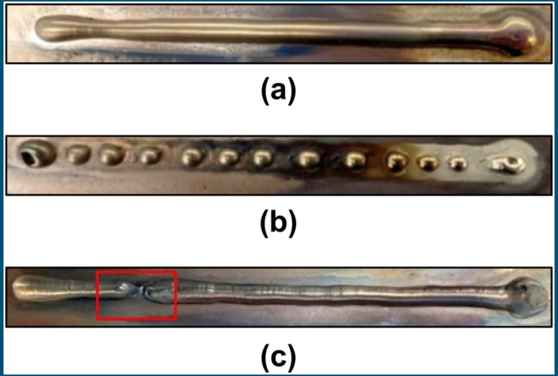
Villarreal, et. al. CMAME 2023

Clustering



L-PBF Metal Properties
Courtesy of Laura Swiler, SNL

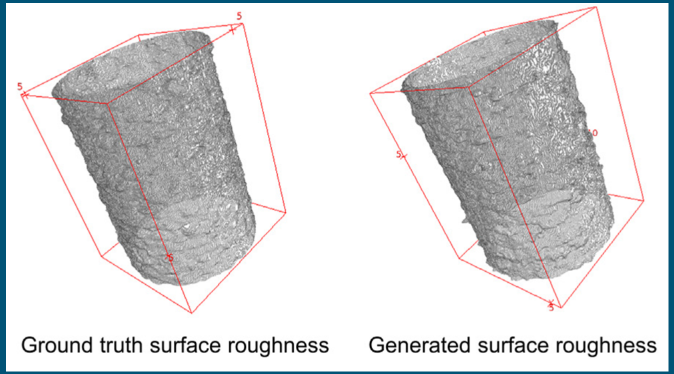
Anomaly Detection



WAAM Build Defects

Cho, et. al. J. Mater Process Tech, 2022

Data Generation



L-PBF Surface

Ogoke, et. al. Additive Manufacturing 2022

Many ML Methods (and Counting)

- Decision Trees
- Neural Networks
- Support Vector Machines
- Genetic Algorithms
- Bayesian Methods
- K-means Clustering
- Random Forest Algorithms

Common Features of ML Approaches

Data / Experience

$X = \{x_1, x_2, \ldots, x_n\}$		Y

Model

$$Y=f(x)$$

Loss Function

$$\varepsilon = \frac{1}{N}\sum_{i=0}^{n} g(f(x_i) - Y_i)$$

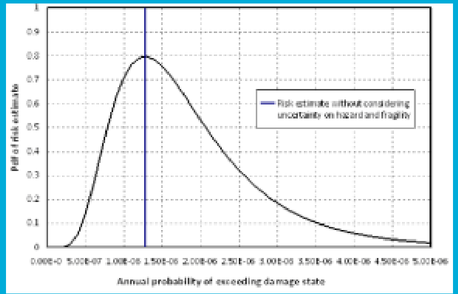
Learning Algorithm

```
if (settings[0].compareTo("s")==0)  {
    if (name.compareTo("") !=0) {
        name += "_";
    }
    name+- etr.getString(settings[1]);
} else if (setting [0].compareTo("d") == 0){
    if (name.compareTo("") !=0) {
        name += "_";
    }
    name += DateUtils.format(etr.getDate(settings[1])
} else if (setting [0].compareTo("d") == 0){
    if (name.compareTo("") !=0) {
        name += "_";
    }
```

Parameterized Model

$$f(x) = \theta_1 x_1 + \theta_2 x_2 + \cdots$$

Predictions & Evaluation



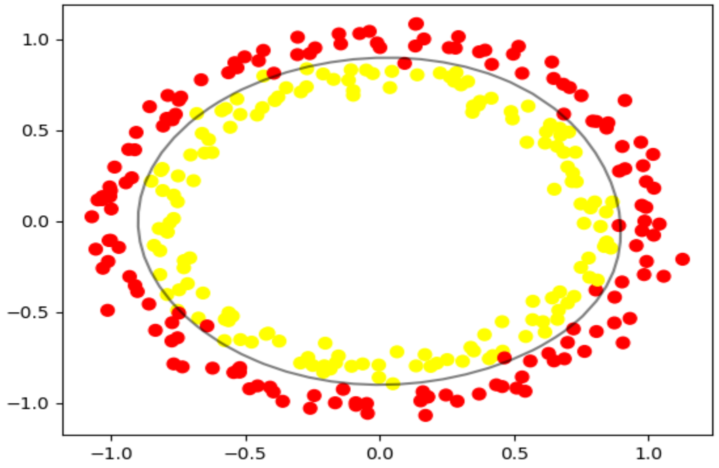
Common Terminology

Loss Function	• Performance metric (notion of error between data and output)
Epoch	• Number of cycles the algorithm takes during training
Training Data	• Data used to train the ML algorithm parameters
Validation Data	• Data used to tune hyperparameters of the algorithm (e.g. number of hidden layers in the neural network)
Test Data	• Data not used during training or tuning that is used to evaluate the error of the trained ML algorithm

Common Algorithms:
Support Vector Machine (SVM) and K-Means Clustering

SVM

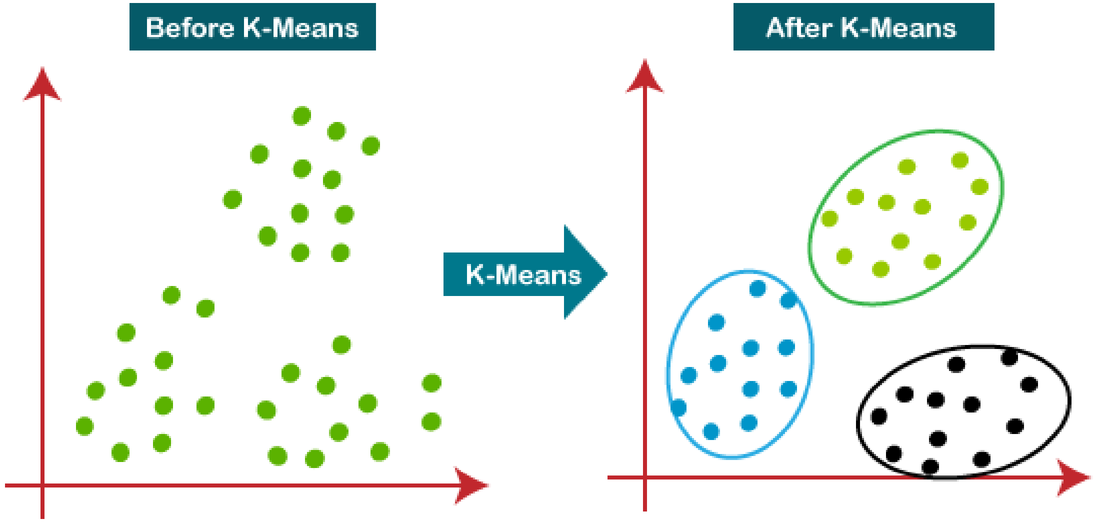
- Finding the "decision boundary" that maximizes the distance from the nearest data points of all the classes
- Can be linear or nonlinear (using kernels)
- Supervised learning



https://www.freecodecamp.org/news/svm-machine-learning-tutorial-what-is-the-support-vector-machine-algorithm-explained-with-code-examples/#:~:text=SVMs%20are%20used%20in%20applications,use%20SVMs%20in%20machine%20learning.

K-Means Clustering

- Grouping similar data points together in k-number of clusters as to minimize the distance of each point to the centroid of a cluster
- The number of clusters k is a hyperparameter
- Unsupervised learning

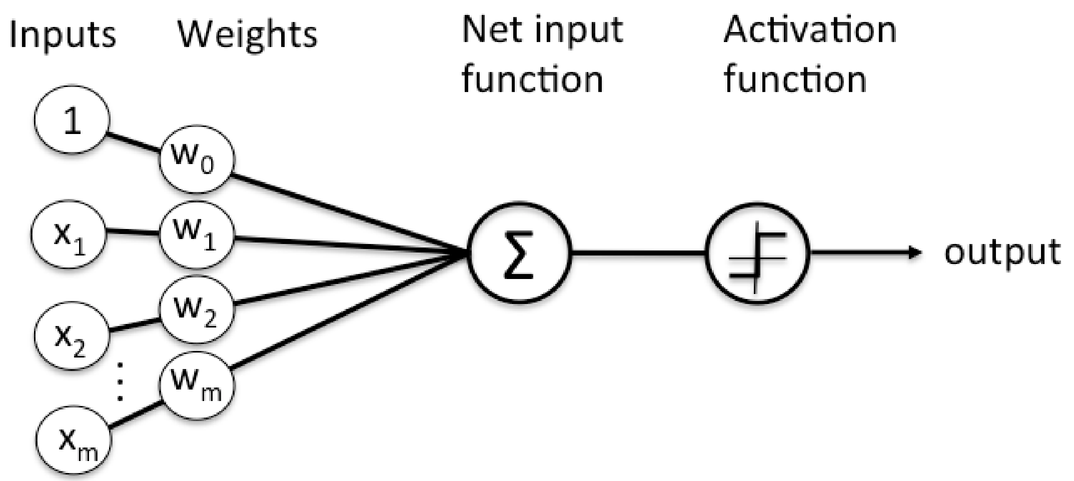


https://www.javatpoint.com/k-means-clustering-algorithm-in-machine-learning

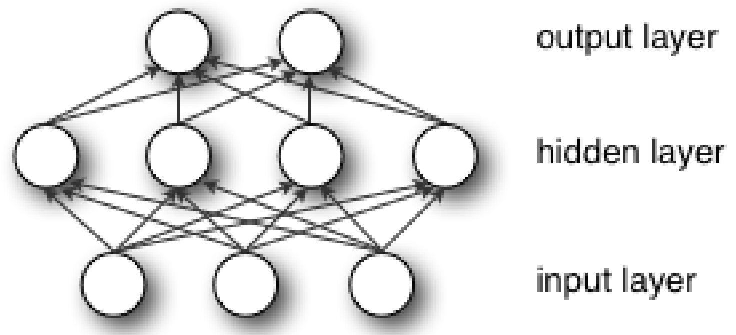
Common Algorithms: Artificial Neural Networks

- A collection of neurons / nodes / perceptrons that each evaluate their local inputs and provides an output evaluation
- Terms:
  - Weights: relative importance of an input
  - Net Input function: sum of the weighted inputs
  - Activation function: evaluates the input for an output (could be evaluated to 0)
  - Layer: collection of nodes
  - Hidden layer: the layers between the input and out layers
  - Deep NN: more than three layers (including the input and output layers)
  - Bias: a node added to each layer to correct systematic biases; only one per layer; a tuned parameter
- Supervised learning, but can be a element of a reinforcement learning algorithm

Single Perceptron / Node / Neuron



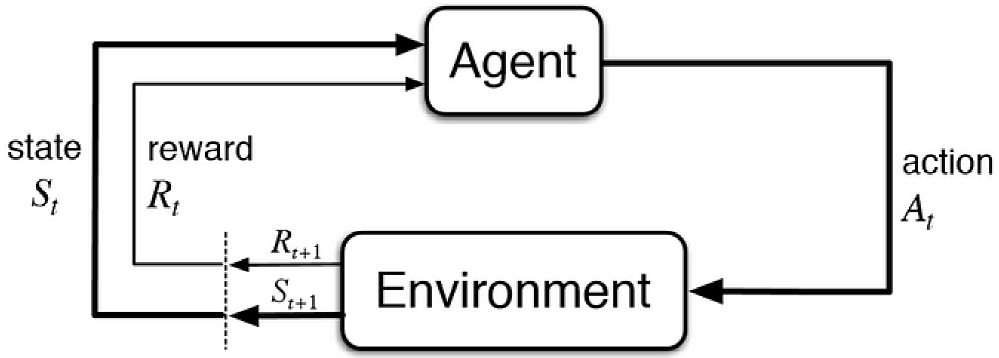
Neural Network

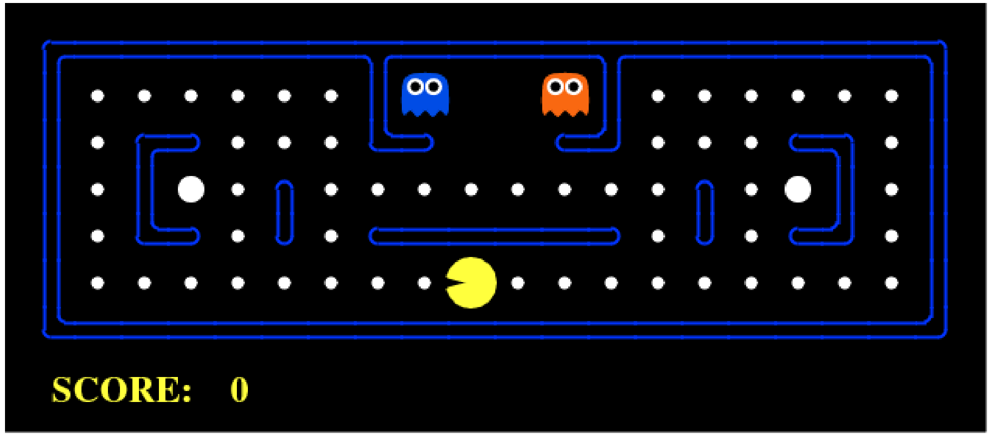


http://wiki.pathmind.com/neural-network#define

Common Algorithms: Reinforcement Learning

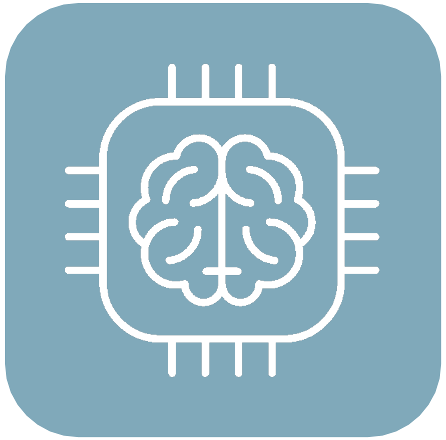
- An Agent interacting with an Environment in a trial-and-error fashion to learn the outcomes or State from Actions to maximize a Reward
- Terms:
  - Environment — Physical world in which the agent operates
  - State — Current situation of the agent
  - Reward — Feedback from the environment
  - Policy — Method to map agent's state to actions
  - Value — Future reward that an agent would receive by taking an action in a particular state
- Exploration vs Exploitation: When training the policy, the agent must balance the exploring new actions with trying to maximize the reward. Short-term sacrifices for long-term reward.



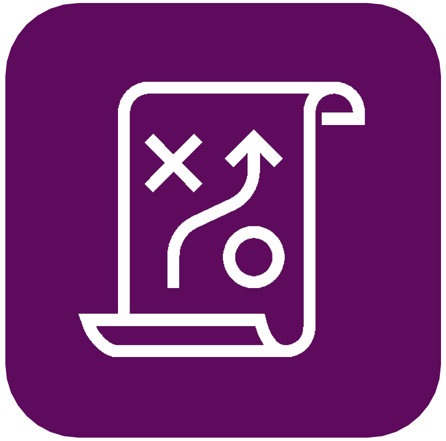


https://towardsdatascience.com/reinforcement-learning-101-e24b50e1d292

Introduction to ML for Mechanics Topics



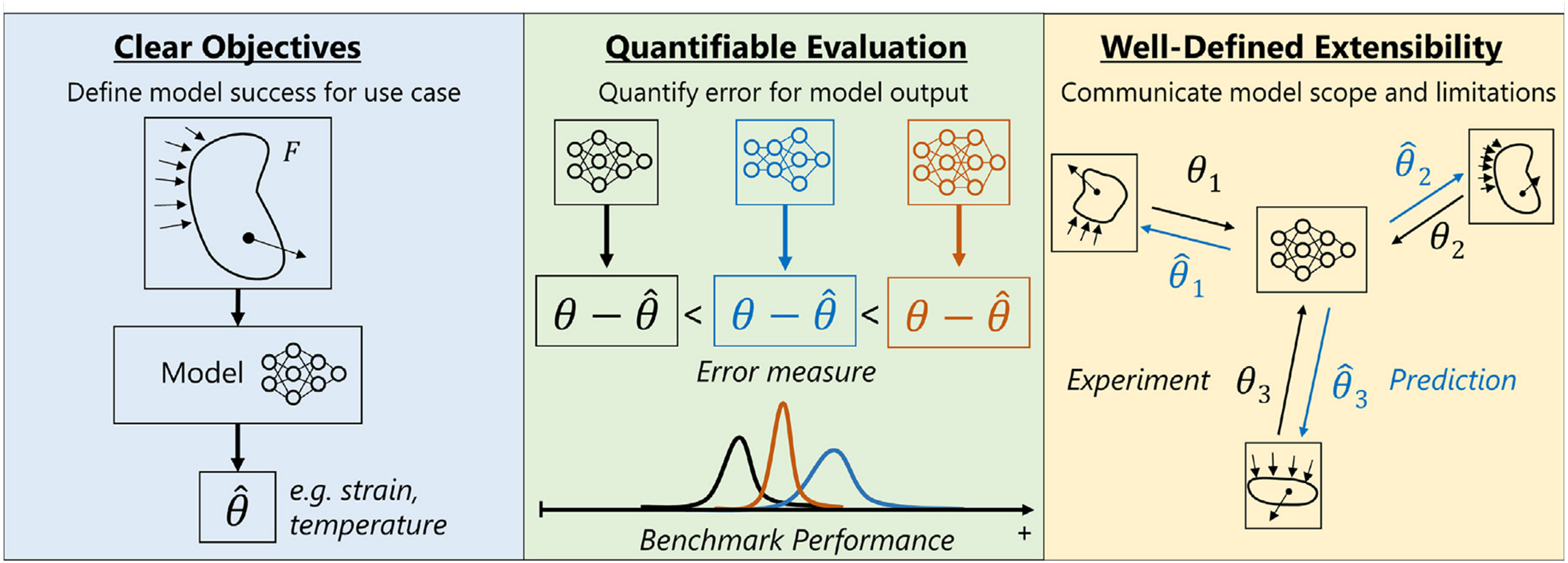
Basic Terms and ML Tasks



Evaluation Approaches

Mechanics Example

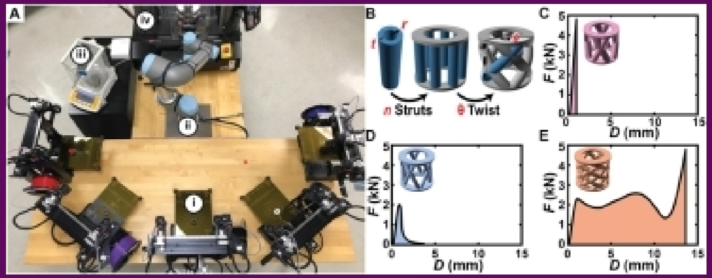
Best Practices in ML in Mechanics



Brodnik, et. al. “Perspective: Machine learning in experimental solid mechanics.” JMPS (2023).

Common Objectives in Mechanics

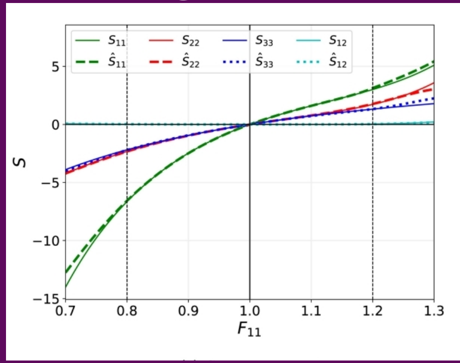
Process Refinement



Automated Testing of AM Structures

Gongora, et. al. Science Advances 2020

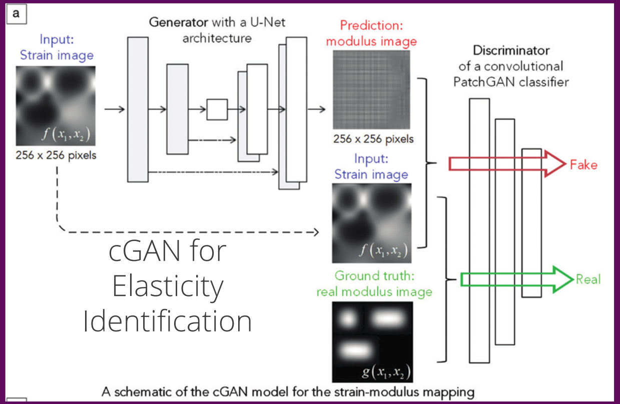
Surrogate Models



Anisotropic Hyperelasticity Using Tensor-Basis NN

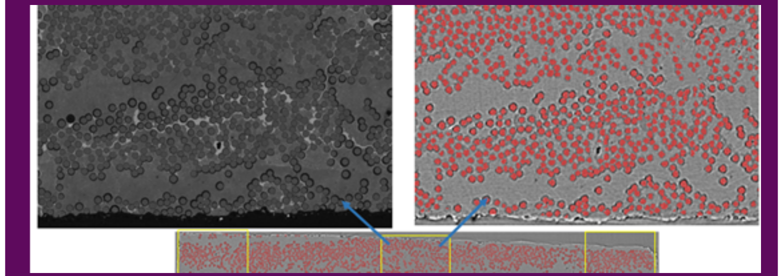
Fuhg, et. al. JMPS 2022

Inverse Problems



Ni and Gao. MRS Bulletin 2021

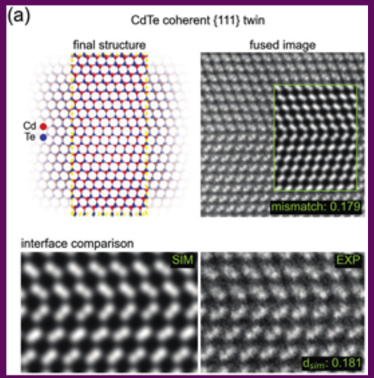
Experiment Augmentation



Identification of Fibers in Composites

Badran, et. al. J Compos. Sci, 2021

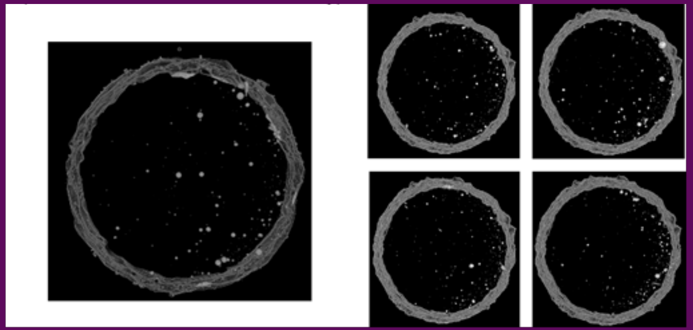
Cross-Measurement Correlation



Fusing Simulations with Experiments

Schwenker, et. al. J. Small, 2022

Data Generation



Original

Synthetic

L-PBF surface and Internal Voids

Ogoke, et. al. Additive Manufacturing 2022

Quantifiable Evaluation

Suitable Error Metrics

Error Against Ground Truth If Possible

Metric Should Quantify the Objective

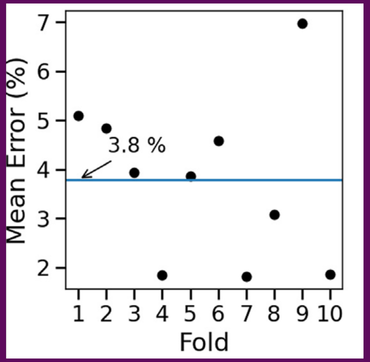
Hold-Out

Training-Validation-Test

Error Metric

Cross-Validation

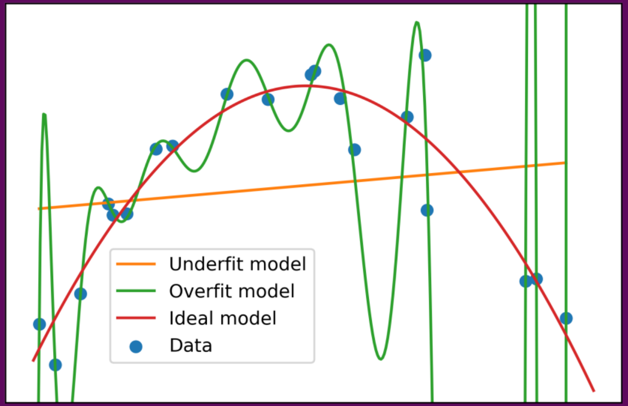
$$LOOCV = \frac{1}{n}\sum_{i=1}^{n} MSE_i$$



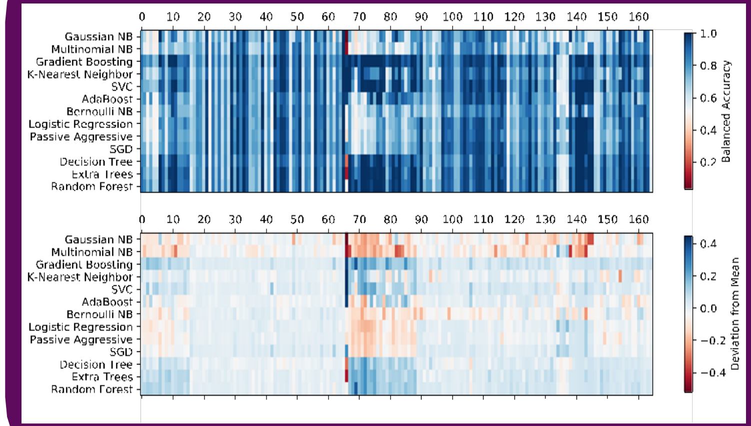
Bootstrap

Distinct Bootstrap Datasets Sampled with Replacement Created and Used to Train the Model. Then the Original Dataset is Used to Test the Model for Error.

Bias and Overfitting



Benchmarking Needed



Olson, et. al. BioData Mining 2017

Well-Defined Extensibility

Model Scope

What salient features of the training data bound the use of the ML model? Extrapolation vs. Interpolation

Knowledge Transfer

Pre-training / Re-training and transfer learning may enable use of an existing ML model with additional data of a similar type to update the model.

Introduction to ML for Mechanics Topics

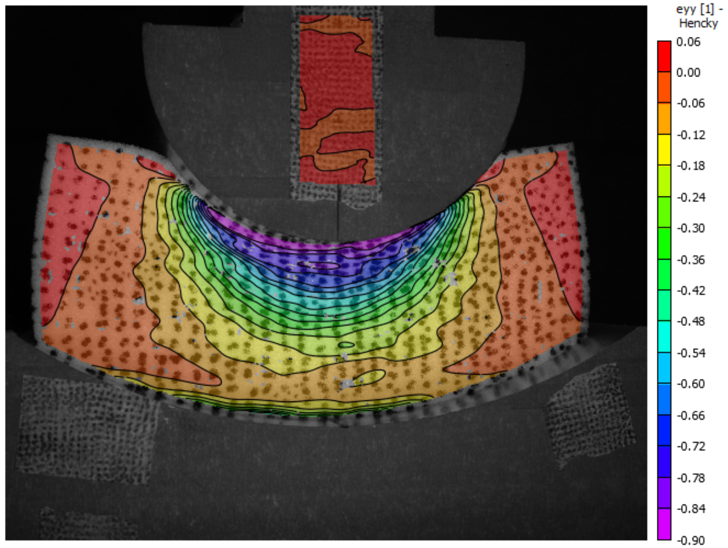
Basic Terms and ML Tasks

Evaluation Approaches

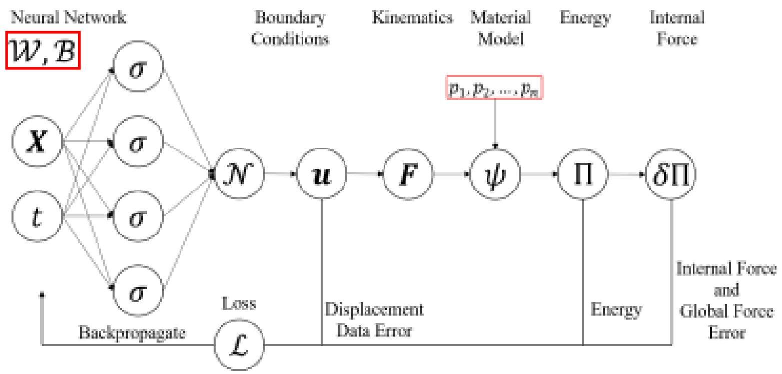
Mechanics Example

Using Physics-Informed Neural Networks (PINNs) to Calibrate Material Models with Full-Field Displacement Data

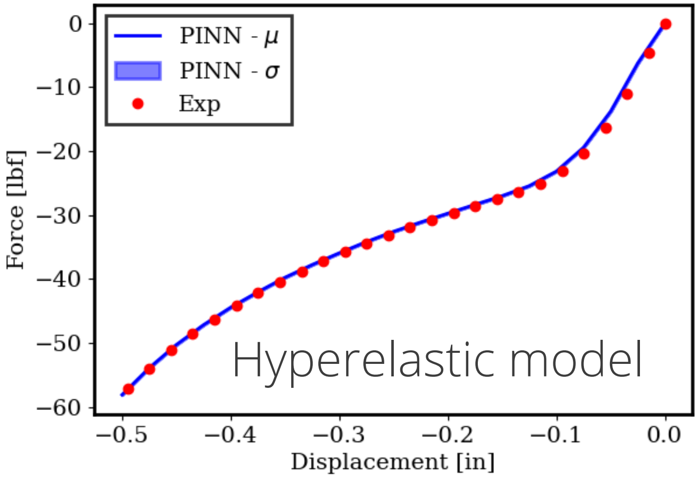
Full-Field Displacement Data



PINN Architecture



$$\psi^{eq}(\lambda_1, \lambda_2, \lambda_3) = \sum^{N} \frac{2\mu_i}{\alpha_i^2}\left[\lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3 + \frac{1}{\beta_i}\left(J^{-\alpha_i\beta_i} - 1\right)\right]$$



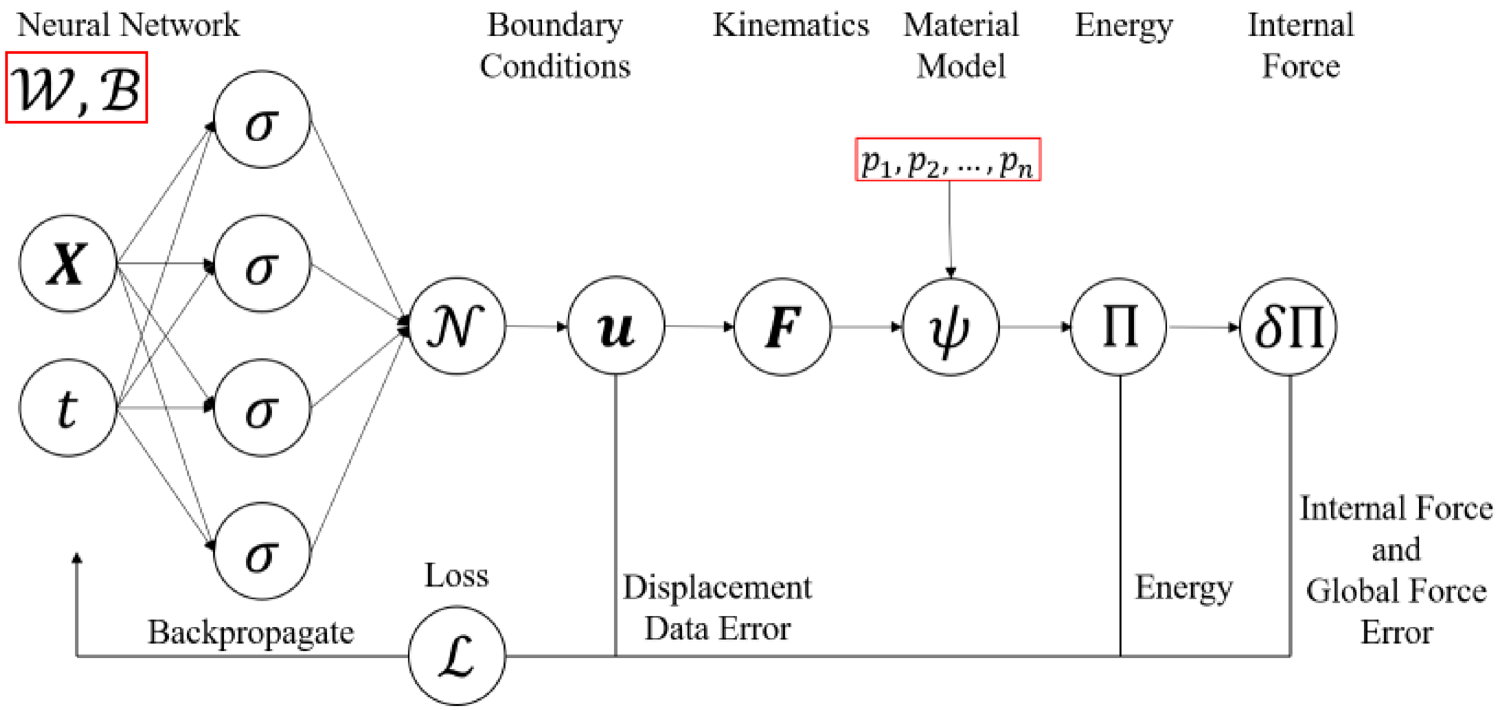
Objective for PINNs:
Inverse problem of calibrating hyperelastic models using full-field surface displacement data and global force-displacement measurements while satisfying kinematics and energy balance

Craig M. Hamel, Kevin N. Long, and Sharlotte L.B. Kramer, "**Calibrating Constitutive Models with Full Field Data via Physics Informed Neural Networks,**" special issue of Strain ("New Trends in Machine Learning, Data-Driven Approaches, and High Performance Computing for Experimental Mechanics"), http://doi.org/10.1111/str.12431

PINNs Architecture That Is Constrained by Mechanics

Strain energy — Energy due to body forces — Energy due to surface tractions

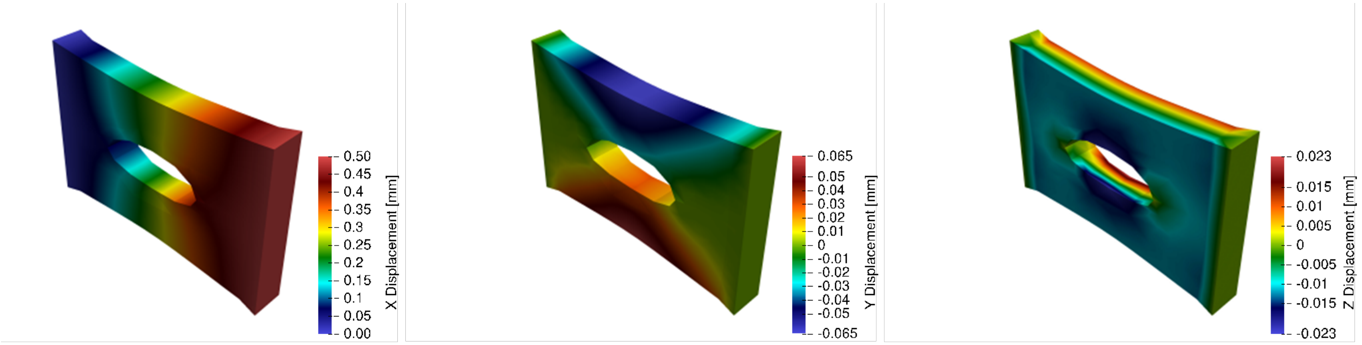
$$\min_{\mathbf{u}\in H^1(\mathcal{B}_0)} \Pi(\mathbf{u}) \longrightarrow \delta\Pi = \int_{\mathcal{B}_0} \delta\psi(\mathbf{E})\, dv - \int_{\mathcal{B}_0} \mathbf{b}\cdot\delta\mathbf{u} dv - \int_{\partial\mathcal{B}_0^{\mathbf{t}}} \tilde{\mathbf{t}}\cdot\delta\mathbf{u} da = 0,$$



Trainable parameters

Benchmarking Performance Against Synthetic Data

Synthetic FEM Training Data:
Only Surface DIC-like Data Used along with
Global Force-Displacement

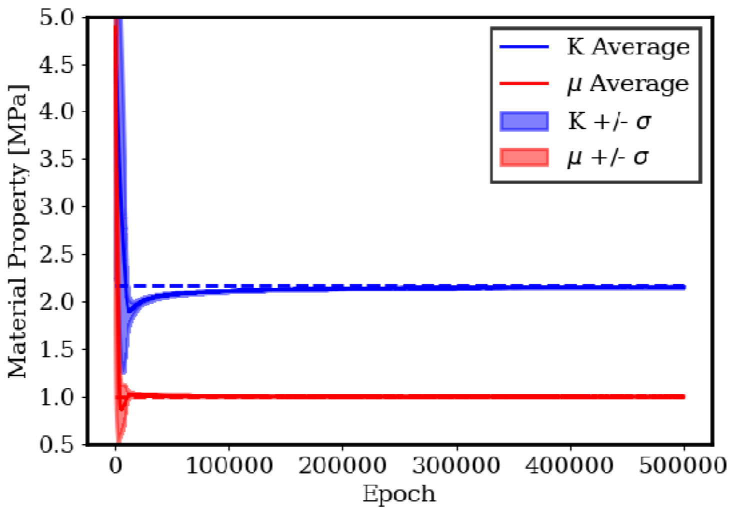


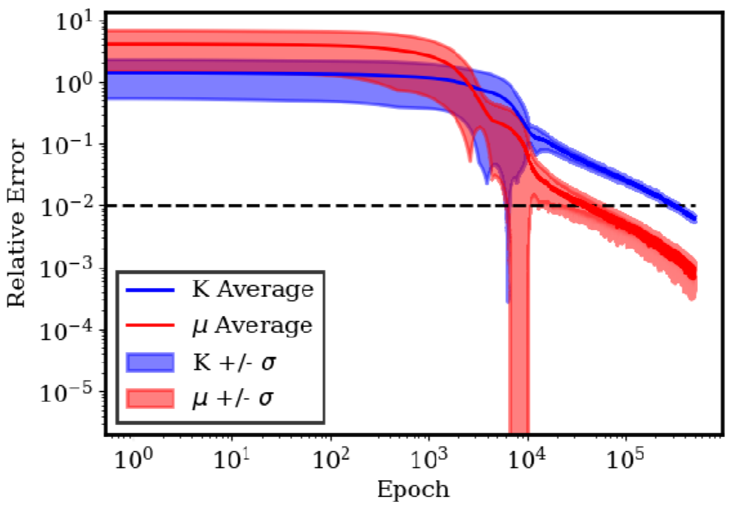
(a) FEM u_x (b) FEM u_y (c) FEM u_z

Neo-Hookean Model with
Bulk and Shear Moduli, K and μ

$$\psi(\mathbf{C}) = \frac{1}{2} K \left[\frac{1}{2} \left(J^2 - 1 \right) - \ln J \right] + \frac{1}{2} \mu \left(\bar{I}_1 - 3 \right),$$

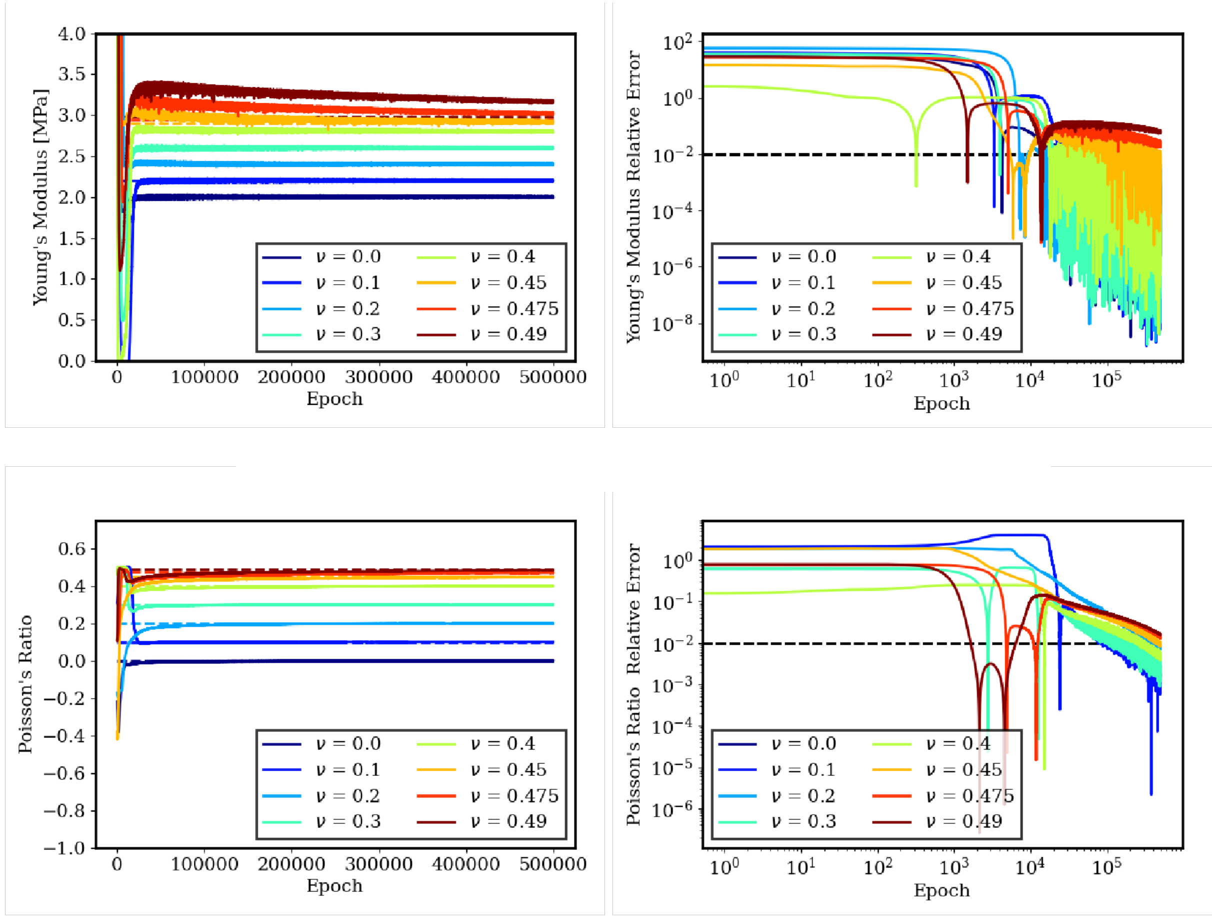
Training and Error (<0.1%)





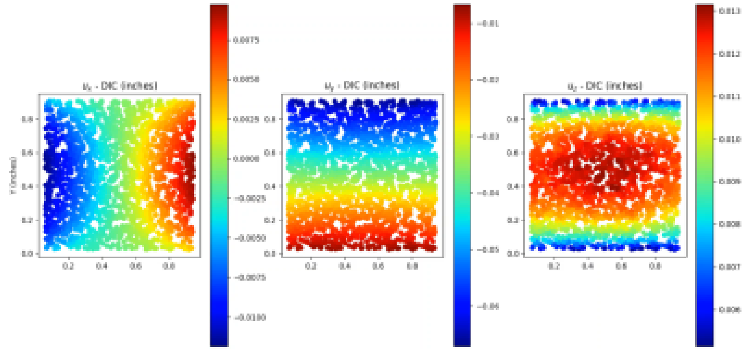
Extensibility of the PINNs Inverse Method

Extensibility to Train for Different Values of Young's Modulus and Poisson's Ratio of a Neo-Hookean Model

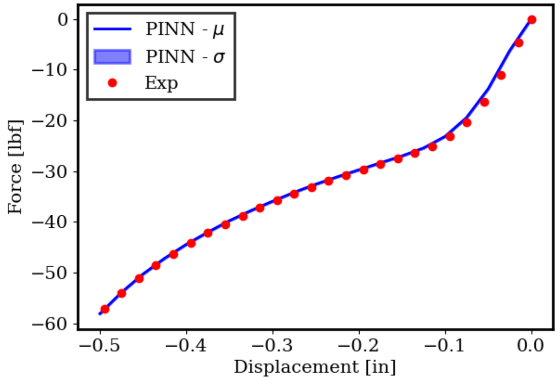


Also tested with Blatz-Ko and Gent Models

Calibration with Experimental DIC Data of Foam Under Compression



Here, **~5% of the correlated DIC points are picked at random for each image** and fed into the PINN along with the global force-displacement data.



Hyperfoam Model for this Polyurethane Foam

$$\psi^{eq}\left(\lambda_1, \lambda_2, \lambda_3\right) = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i^2} \left[\lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3 + \frac{1}{\beta_i}\left(J^{-\alpha_i \beta_i} - 1\right)\right]$$

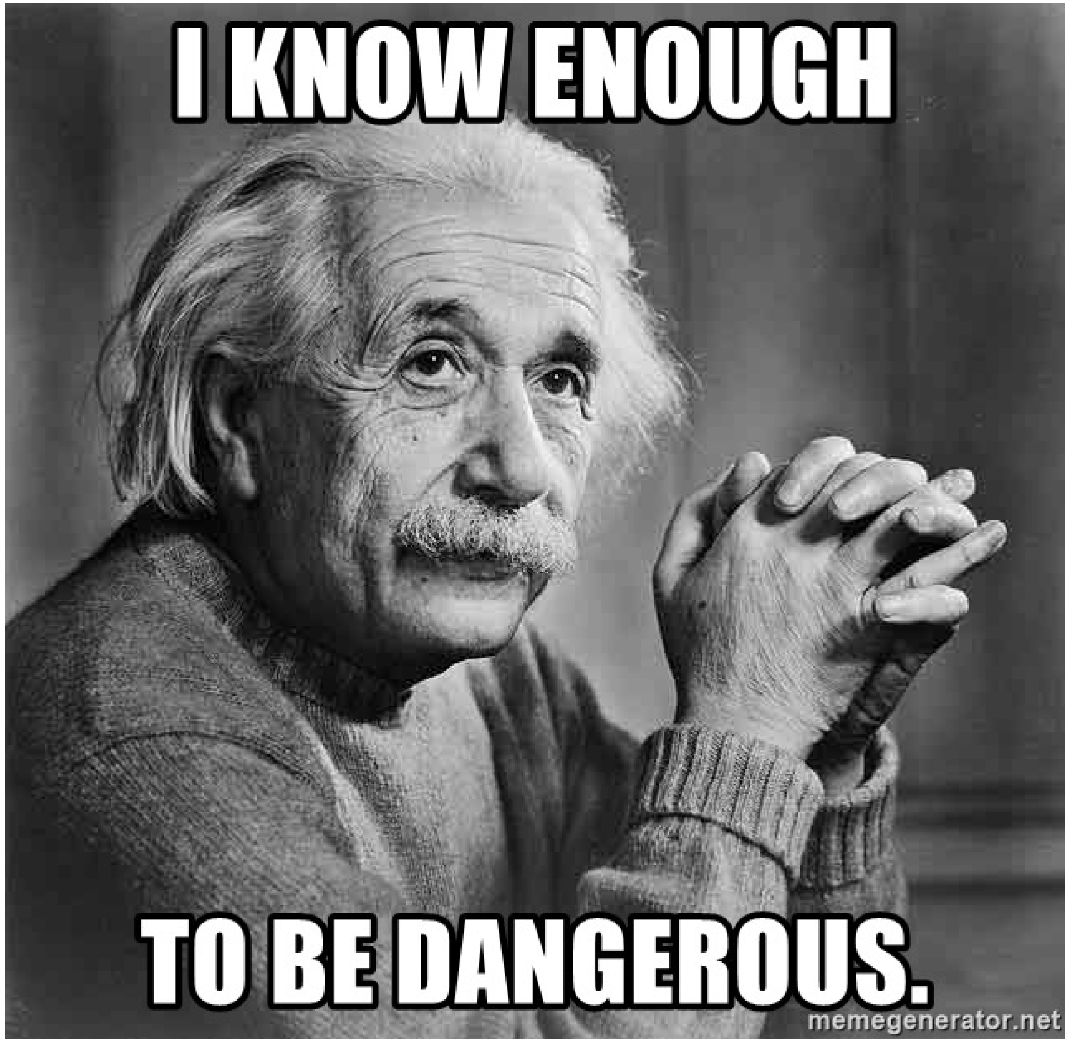
A Brief Introduction to ML for Mechanics

Basic Terms and ML Tasks

Evaluation Approaches

Mechanics Example

Thanks for your attention!



https://www.solidsmack.com/engineering/things-to-stop-saying-i-know-enough-to-be-dangerous/

Backups

Our PINNs approach to material model calibration utilizes heterogenous full-field data and global force data.

Kinematics

Displacement BC

Neural network

$$\mathbf{u}_{\mathcal{N}}(\mathbf{X},t) \approx \tilde{\mathbf{u}}(\mathbf{X},t) + f(\mathbf{X})\,\mathcal{N}(\mathbf{X},t)$$

$$\mathbf{F}^e_{\mathcal{N}} = \mathbf{I} + \nabla_{\mathbf{X}}\mathbf{u}^e_{\mathcal{N}}$$

Standard shape functions for Hex8 elements

$$\nabla_{\mathbf{X}}\mathbf{u}^e_{\mathcal{N}} = \sum_{I=1}^{N_{nodes}} \mathbf{u}^I_{\mathcal{N}} \otimes \nabla_{\mathbf{X}} N^I$$

Total potential energy for time step n

$$\Pi^n_{\mathcal{N}} = \sum_{e=1}^{N_e}\sum_{q=1}^{N_q} w_q\left(\det \mathbf{J}^e\right)\psi^e\left(\mathbf{F}^e_{\mathcal{N}}\right)$$

Internal Force Vector

$$\mathbf{f}_{\mathcal{N}} = \delta\Pi_{\mathcal{N}} = \frac{\partial \Pi_{\mathcal{N}}}{\partial \mathbf{u}_{\mathcal{N}}}$$

Total loss function $\mathcal{L} = \beta\mathcal{L}_r + \gamma\mathcal{L}_{\mathbf{u}} + \delta\mathcal{L}_f$

Loss function for potential energy $\mathcal{L}_r = \Pi_{\mathcal{N}} + \alpha\|\delta\Pi_{\mathcal{N}}\|^2_{free}$

For inverse problems we have the additional error terms for experimental data

Surface Displacements

$$\mathcal{L}_{\mathbf{u}} = \frac{1}{N_{\mathbf{u}}}\sum_{i=1}^{N_{\mathbf{u}}} \|\mathbf{u}_{\mathcal{N}}\left(\mathbf{X}^*_i, t^*_i\right) - \mathbf{u}^*_i\left(\mathbf{X}^*_i, t^*_i\right)\|^2$$

Global Force

$$\mathcal{L}_f = \frac{1}{N_t}\sum_{n=1}^{N_t} \|f_{net}\left(t_n\right) - f^*_{net}\left(t_n\right)\|^2$$