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Sandia National Laboratories

Integrating Physics through Constrained Machine Learning Loss

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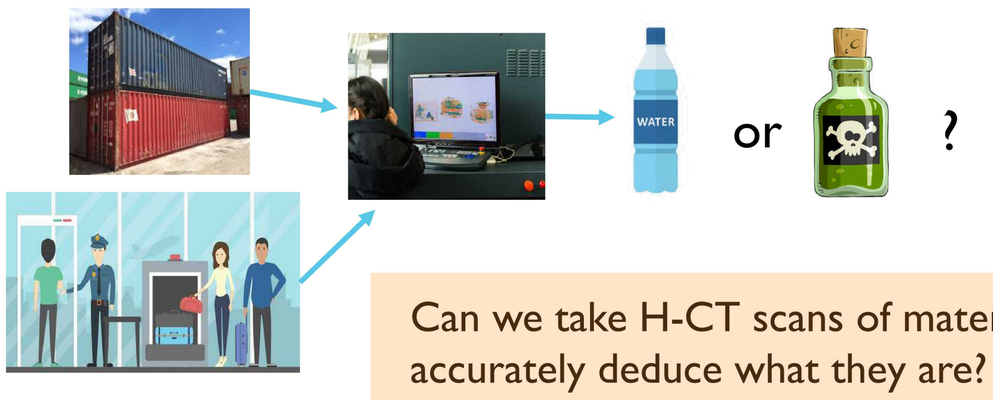
Problem:

Material Classification using hyperspectral-computed tomography (H-CT)



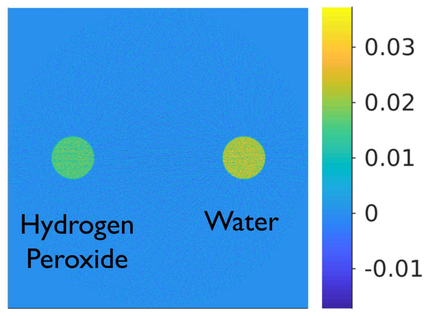
Can we take H-CT scans of materials and accurately deduce what they are?

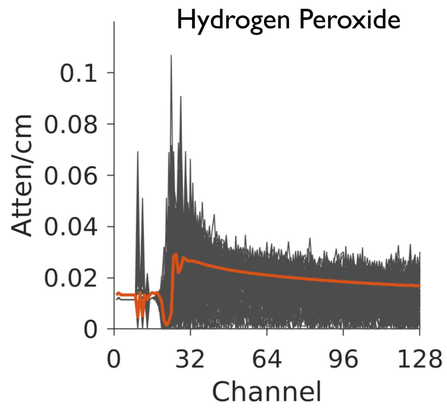
Simulated H-CT Scans

Simulation of data set of difficult to identify materials.

- Water
- Hydrogen peroxide
- Diluted hydrogen peroxide
- Explosive
- Shielded -vs- non-Shielded conditions

Data simulated using Particle and Heavy Ion Transport code System (PHITS).

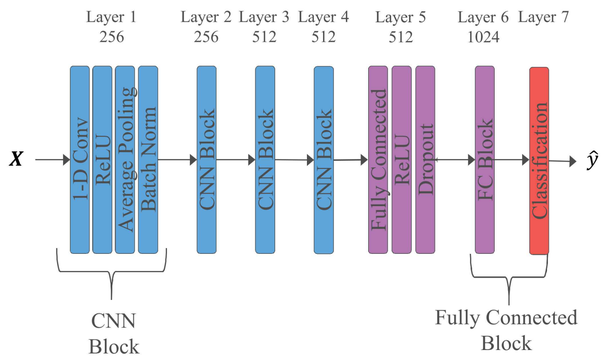


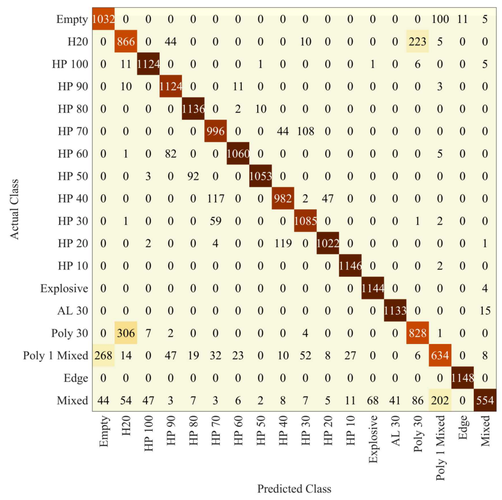


Current Work:

Neural Networks and Functional Data Analysis (FDA) perform material classification on simulated data.

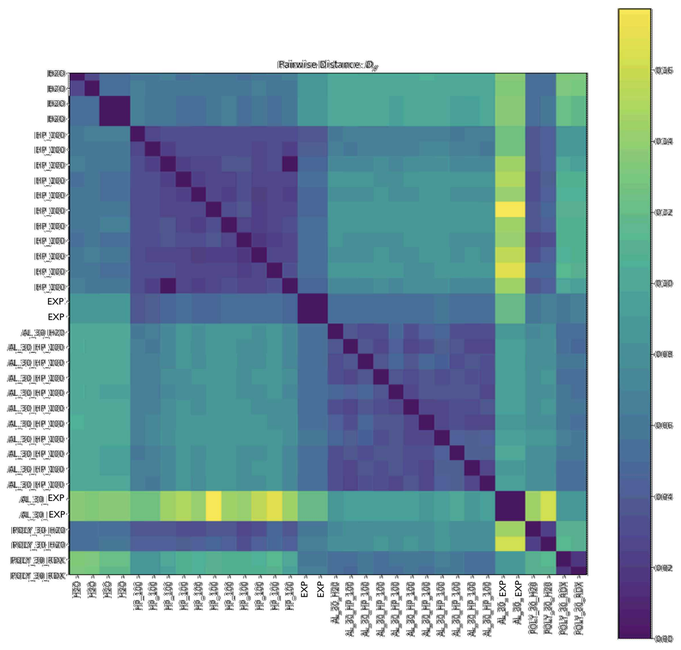
Convolutional Neural Net (CNN)



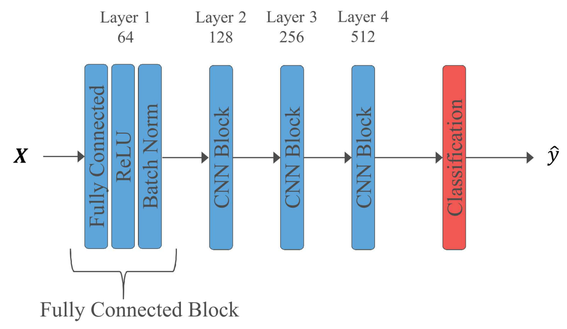


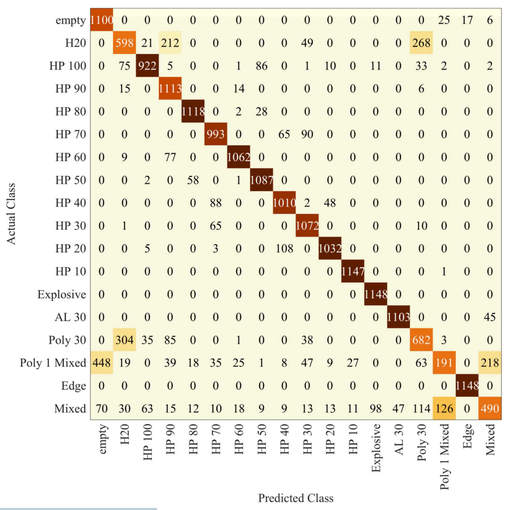
fda: Using a metric that has physical interpretation enables us to measure similarity between curves of different material types.

(Fisher-Rao on squared-velocity space)



Deep Neural Net (DNN)





Question:

Can we improve models by penalizing predictions that don't agree with theory: utilizing the energy dimension available in HC-T?

Ongoing Work:

Take measurements on real materials and integrate simulated attenuation curves using distance-based loss function that encourages classification models to penalize deviance from scientific theory.

$$L_d(y, \hat{y}) + \lambda L_s(f(x), f(x|\hat{y}))$$

'data-driven loss' 'science-driven loss'

$y, \hat{y}$ - true/predicted label
$f(x), f(x|\hat{y})$ - true/predicted attenuation curve
λ - penalty for prediction deviating from theory

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