Deep Learning for Elemental Mass Quantification using Spectral X-Ray Radiography

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Overview

1. Introduction
2. Spectral X-Ray Radiography
3. Convolutional Neural Networks
4. Dataset Synthesis
5. Results and Conclusion

[1] “The Invisible” (1896)
Objective of this work

- Use deep learning to predict mass of each element present in a sample from spectral radiograph within 1% relative error
  - Test Case: Bi$_2$O$_3$ powder
X-Ray Radiography

Typical Planar Configuration:


Energy-Sensitive, Pixelated Detectors

Readout board for LETI linear CdTe detector [6]

HEXITEC [4]

Medipix2 array detector [5]
Spectral X-Ray Radiography

\[ \Phi(E) = \Phi_0(E) e^{-\sum_k \mu_k(E) x_k} + \Phi_{scatt} \]

- **Initial Spectrum**
- **Attenuation Coefficients**
- **Solve for** \( x_k \)
  - Presence: Material Discrimination
  - Amount: Mass Quantification


Numerical Approaches

\[ \Phi(E) = \Phi_0(E) e^{-\sum_k \left( \frac{\mu}{\rho} \right)_k (\rho_A)_k} \]

\[ T(E) = \frac{\Phi(E)}{\Phi_0(E)} \]

\[ -\ln T(E) = \sum_k \left( \frac{\mu}{\rho} \right)_k (\rho_A)_k \]

\[ r_i = \int_{E_i} -\ln T(E) \, dE \]

\[ \tilde{r} = A \tilde{\rho}_A \]

\[ \tilde{\rho}_A = (A^T A)^{-1} A^T \tilde{r} \]

Sandia for explosives detection

- Apply Simplex Method by approximating energy dependence with Legendre polynomials
- Performed CT reconstruction


PNNL for Safeguards

- Apply Quadratic Method: Non-linear least-squares
- Used non-negativity constrained Gauss-Newton method with reduced Hessian

Experimental Setup

X-RAY SOURCE

SAMPLE

DETECTOR
Experimental Setup

X-RAY SOURCE

SAMPLE

DETECTOR
Experimental Spectral Radiographic Data

Energy-Integrated Image
Propose Convolutional Neural Networks

- First shown to thrive in image classification
- Uses notion of “filter” instead of normal connections
- Extracts “spatially” relevant features/patterns in data
- Not just limited to space. Now used for temporal, etc.

3D CNNs

- Spectral radiograph has 2 spatial, 1 energy dimension
- ResNet-34

What about the data?

- Deep learning needs thousands or millions of training examples

<table>
<thead>
<tr>
<th>Experimental Data</th>
<th>Simulated Data</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pros:</strong></td>
<td><strong>Pros:</strong></td>
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<tr>
<td>• Training set is representative of what it is trying to learn</td>
<td>• Inexpensive</td>
</tr>
<tr>
<td>• No required post-processing (though may be useful)</td>
<td>• Know mass perfectly</td>
</tr>
<tr>
<td></td>
<td>• Ability to add variation and expand dataset</td>
</tr>
<tr>
<td><strong>Cons:</strong></td>
<td><strong>Cons:</strong></td>
</tr>
<tr>
<td>• How well is the mass really understood?</td>
<td>• Not necessarily reflective of reality</td>
</tr>
<tr>
<td>• Time consuming</td>
<td></td>
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<tr>
<td>• Need diversity of examples</td>
<td></td>
</tr>
</tbody>
</table>
Examples of dataset

\[ \Phi(E) \]

\[ 1 - \frac{\Phi(E)}{\Phi_0(E)} \]
Examples of dataset

Training and Validation Results: 1800 s

\[
\text{Rel. Error} = \frac{\hat{y} - y}{y}
\]

\(\hat{y}\): calculated from network

\(y\): ground truth
Relative Error Distribution on Test Dataset
Conclusion

• Presented DL approach to mass quantification
  ▪ Synthesized dataset using Monte Carlo
  ▪ Transformed simulations via augmentation, DRF, noise
  ▪ Applied 3D ResNet-34 CNN to predict mass
  ▪ Tested on 4 acquisition durations

• Capable of average performance < 1% test error
  ▪ Longer acquisitions gave had tighter distributions
Future Work

DEAD PIXELS
EFFICIENCY

X-RAY FLUORESCENCE

DOMAIN ADAPTATION

\[
\begin{align*}
\text{DEAD PIXELS} & \quad \text{EFFICIENCY} \\
\text{X-RAY} & \quad \text{FLUORESCENCE} \\
\text{DOMAIN} & \quad \text{ADAPTATION}
\end{align*}
\]
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Thank you
Numerical Approaches: Transmittance Logarithm

Georgia Tech and Penn State

\[
\frac{\ln T(E_1)}{\ln T(E_2)} = \frac{\mu(E_1)}{\mu(E_2)}
\]

ResNet-34

- Skip Connections:
  - Help with vanishing gradient problem
- Adapted to 3D convolutions
- Implemented in TensorFlow
- Input: Spectral Radiograph
- Output: Elemental Mass