OpenAGS: an Analysis Program for Prompt Gamma Activation Spectra

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How PGAA Works

- The sample in question is irradiated using a neutron beam
- Sample nuclei become excited
- Nuclei emit gamma rays upon de-excitation
- The energy of these gamma rays depends on the specific element that produced them
- Several advantages over traditional INAA
- Detects a few specific elements (B, Cd, Sm, Gd) at 10-100 ppb, many others at 1-10 ppm
Project Goals

Current Workflow for PGAA Data Analysis:

1. Isotope(s) Sensitivity Table
2. Create ROIs in acceptable format (R Script)
3. Spectrum File → Peak Fitter (PeakEasy)
4. Convert Peak Areas to Element Masses (R script)
5. Output File
Project Goals

Planned Workflow:

1. Spectrum File(s) Elements of Interest
2. GUI Program
3. Masses (grams and moles) of elements of interest (csv file)
Finding Elemental Mass from Data

- Plot counts per second as a function of energy
- Look for peaks at predetermined locations
- Find area under peak (A)
- Sensitivities (S) have already been determined by irradiating a known amount of the target element (S = A/mass)
- Mass = A/S
- So given a peak with area 20 cps and sensitivity 2 cps/mg, we can determine that there are 10 mg of the associated element in the sample
Finding the True Area of Peaks

- Overlapping Peaks
- Background Noise
- Peaks not in predictions library
- Solution: Nonlinear Least-Squares Fitting
Gaussian Peaks and why they Matter

- Like Normal distributions, but area underneath can be any value
- Caused by detector response to gamma rays at a single frequency (the center)
- Overall equation to model multiple peaks

\[ a e^{-\frac{(x-b)^2}{2c^2}} \]
My Approach to the Problem

- Find local maxima
- Guess initial parameters for Gaussians
- Guess the equation of a line that models background data
- Use a curve fitter (scipy.curve_fit) to optimize my guesses
- Match peaks to isotopes
- Divide by sensitivity, and output the mass
Live Demo
## Comparison With Existing Solution

<table>
<thead>
<tr>
<th>Software</th>
<th>Integration</th>
<th>Proprietary Software</th>
<th>Time for Setup</th>
<th>Batch Processing</th>
<th>ROI Editing</th>
<th>Peak Fitting</th>
</tr>
</thead>
<tbody>
<tr>
<td>Existing Solution (R Code and PeakEasy)</td>
<td>3 steps, several intermediate files</td>
<td>PeakEasy, closed source and only available to US Government</td>
<td>10-30min</td>
<td>Yes</td>
<td>Simultaneous, can manually adjust region</td>
<td>Predetermined fit with 1-2 Gaussians</td>
</tr>
<tr>
<td>OpenAGS</td>
<td>1 step</td>
<td>None</td>
<td>Comparable</td>
<td>Yes</td>
<td>Sequential, can manually adjust region and add/remove Gaussians</td>
<td>Fits multiple Gaussians and background line</td>
</tr>
</tbody>
</table>

### Comparison of Masses Calculated

![Comparison of Masses Calculated](image)

- **Current Solution (PeakEasy and R code)**
- **OpenAGS**
Future Work

- Present more data to the user during the analysis process
- Fit Doppler-Broadened Gaussians like the B-11 peak
- Add support for more complex functions to model the Detector Response
- Add a feature which allows the user to calculate sensitivities from spectra created by irradiating known masses
Questions?