Automated Variable Selection of Gamma-Ray Responses by Utilizing LASSO and Elastic Net

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Agenda

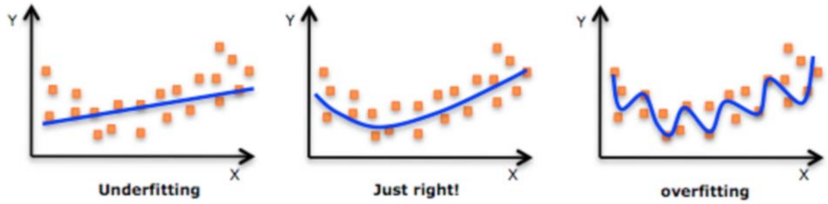
- Monte Carlo Library Least Squares (MCLLS) fitting
- Basics of supervised machine learning
- Regularization methods (LASSO and Elastic Net)
- Prompt Gamma Neutron Activation Analysis (PGNAA)
- Library generation and data processing
- Results

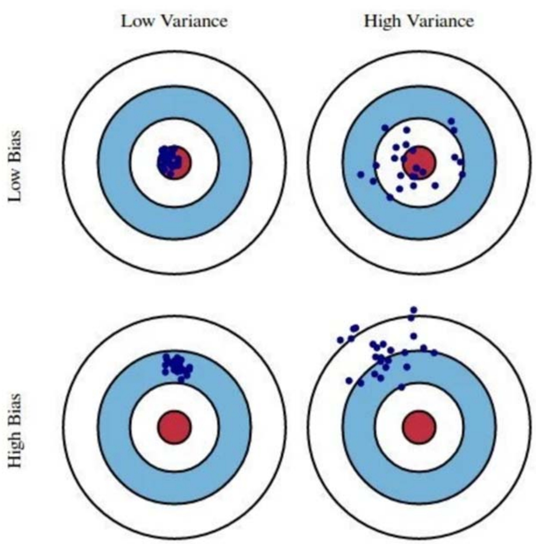
Monte Carlo Library Least Squares

- Same principle as ordinary least squares with library spectra used as the input
- $y_i = \sum_{j=1}^{m} x_j a_{ij} + E_i, i = 1, n$
  - y_i is the counts per channel i
  - x_j are linear coefficients for each element j
  - a_{ij} are the library spectra, or counts in channel i of element j
  - E_i is random error in counts in channel i
- How to deal with changing environments and unknown compositions?

Supervised Machine Learning

- Ordinary Least Squares traditionally suffers from overfitting
  - Too many model parameters
- Model selection should have the right parameters to accurately predict/fit correct solution
- Adding complexity to the model increases bias while reducing variance
- Supervised machine learning variable selection techniques aim to minimize unnecessary bias and variance simultaneously by selecting the correct parameters





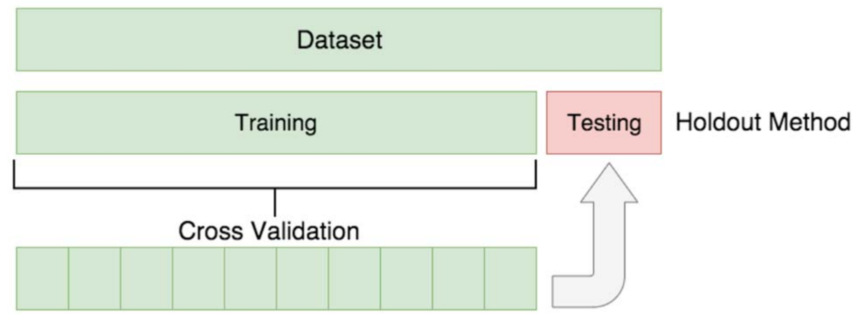
LASSO and Elastic Net

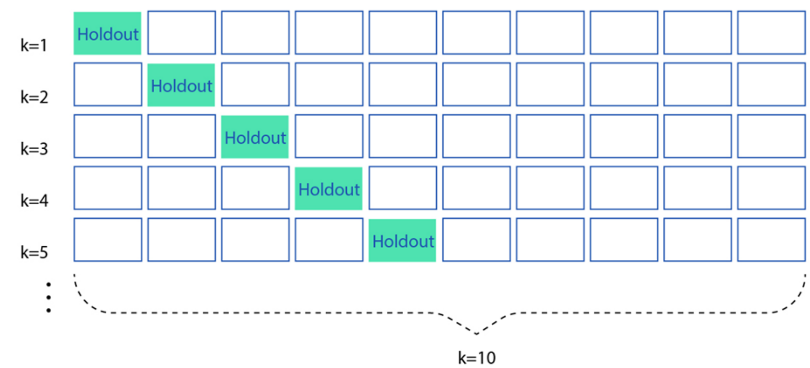
- The LASSO (Least Absolute Selection and Shrinkage Operator) is defined as:
  - $\hat{\beta}^{lasso} = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} ||y - X\beta||_2^2 + \lambda \sum_{j=1}^{p} |\beta_j|$

    or $\quad = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} ||y - X\beta||_2^2 + \lambda||\beta||_1$
  - Where the first term is the loss function and $\lambda||\beta||_1$ serves as a penalty
    - Note: if $\lambda=0$, the equation is identical to that of Ordinary Least Squares (OLS)
- Elastic Net is a modification of LASSO that adds a quadratic penalty as defined below:
  - $\hat{\beta}^{ElasticNet} = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} ||y - X\beta||_2^2 + \lambda_2||\beta||^2 + \lambda_1||\beta||_1$
- As $\lambda_{1,2}$ increase, the penalty for each new coefficient grows, allowing variable selection to occur in linear models

Cross Validation

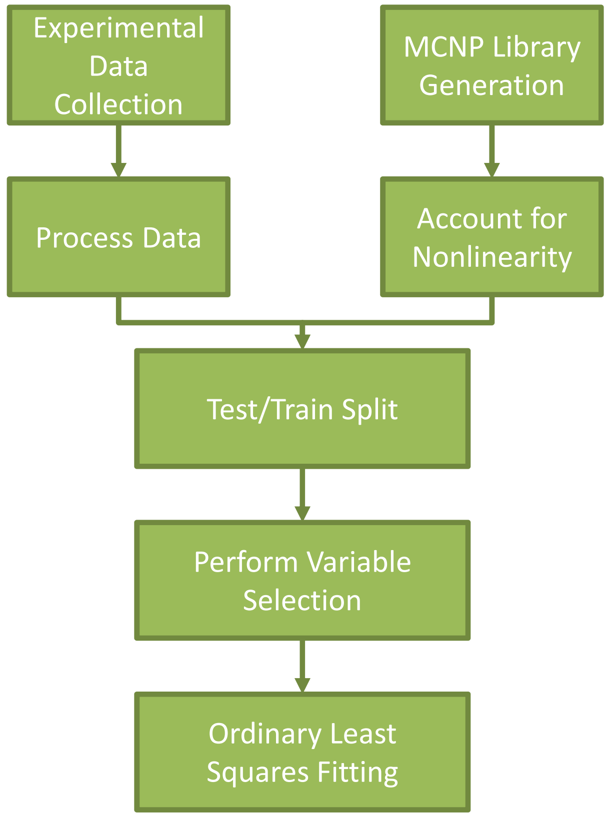
- Each method relies on test/train split to tune model parameters
- This step introduces bias from selecting some data over others (random)
- Cross validation performs the test/train split multiple times, reducing random bias from the model training
  - Trade off - extra computing time





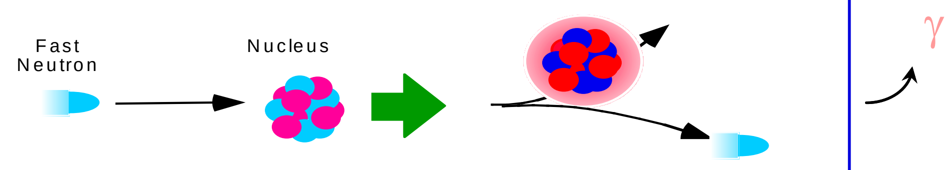
Full Run Flow Chart

- Simulated and experimental data is generated
- Each set is processed
  - Nonlinearities removed
  - Prompt/delayed responses are extracted
- Test/train split data for model selection
- Variable selection through LASSO or Elastic Net remove unnecessary model parameters and provides initial guesses
- Final ordinary least squares fitting to reduce bias from model selection procedure



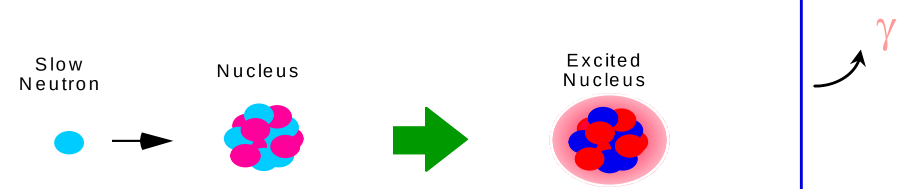
Neutron Interactions

INELASTIC SCATTERING



C, O, Si, Ca, Fe, ...

THERMAL CAPTURE



H, Cl, Si, Ca, S, Fe, Gd, ...

NEUTRON ACTIVATION

Inelastic or capture reaction that leads to a radioactive element and decay.
Examples:

O-activation	$T_{1/2} = 7.1$ s	$(n + {}_{8}O^{16} \rightarrow {}_{7}N^{16} + \ldots \rightarrow {}_{8}O^{16} + \gamma + \ldots)$
Al-activation	$T_{1/2} = 2.3$ m	$(n + {}_{13}Al^{27} \rightarrow {}_{13}Al^{28} \rightarrow {}_{14}Si^{28} + \gamma + \ldots)$
Si-activation	$T_{1/2} = 2.3$ m	$(n + {}_{14}Si^{28} \rightarrow {}_{13}Al^{28} + \ldots \rightarrow {}_{14}Si^{28} + \gamma + \ldots)$

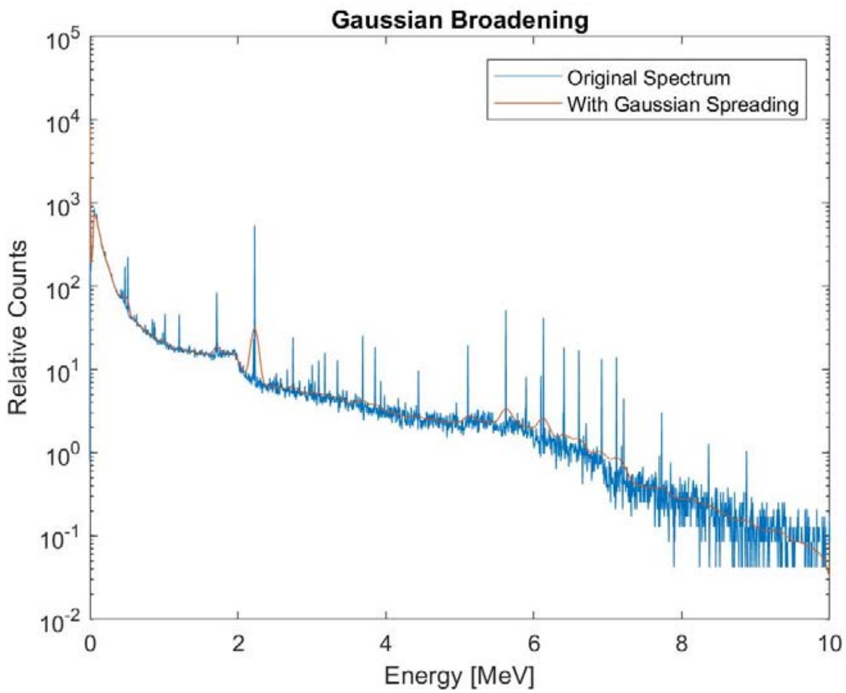
(Na, Cu, Fe..... and many more).

Library Generation

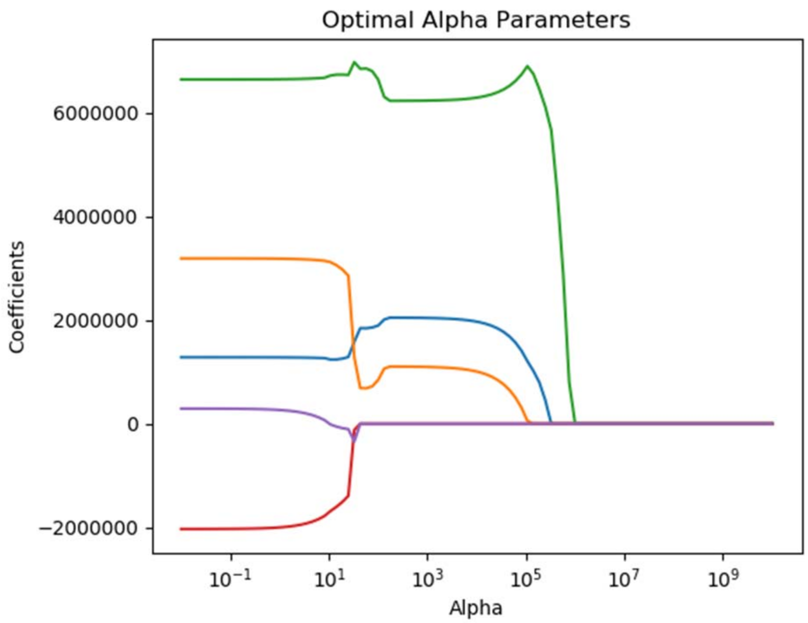
- Extensive MCNP simulations
  - Center for Engineering Applications of Radioisotopes (CEAR) cluster – reduced run times from 1.5-3 days to ~1 hour
  - F8 tally for gamma detection
  - No GEB
- Detector Response Function (DRF)
  - Response generated in a detector from incident radiation
  - Non-linearities resolved to treat problem as a linear combination of library inputs
    - Gaussian broadening fit of full width/half max using calibration sources
    - Energy to channel conversion (2nd order polynomial in the following examples)
      - Both of these will be upgraded by the work performed by Aaron Feinberg

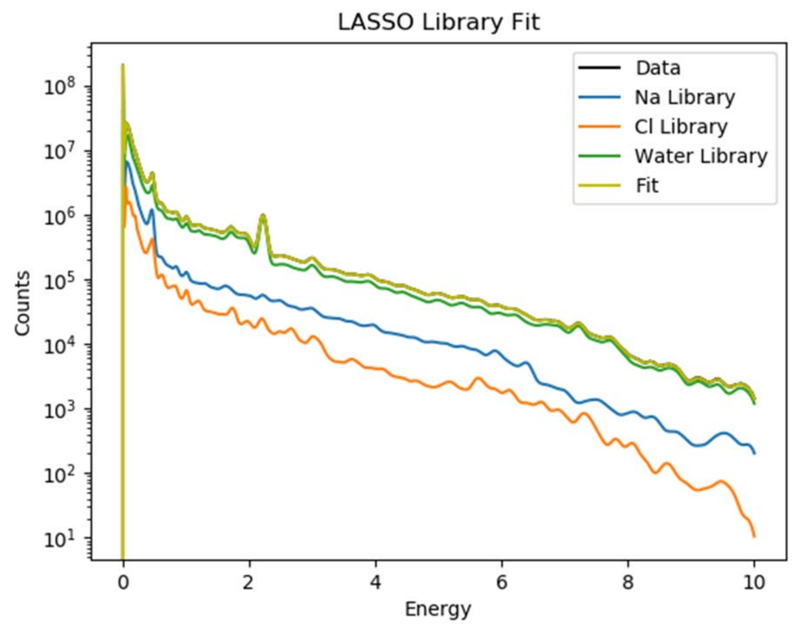
Processing of Data

- MCNP simulations are broadened post processing (faster than GEB tally)
- Nonlinear NaI response requires adjustment during channel to energy conversion
- $Energy = a + b * channel + c * channel^2$



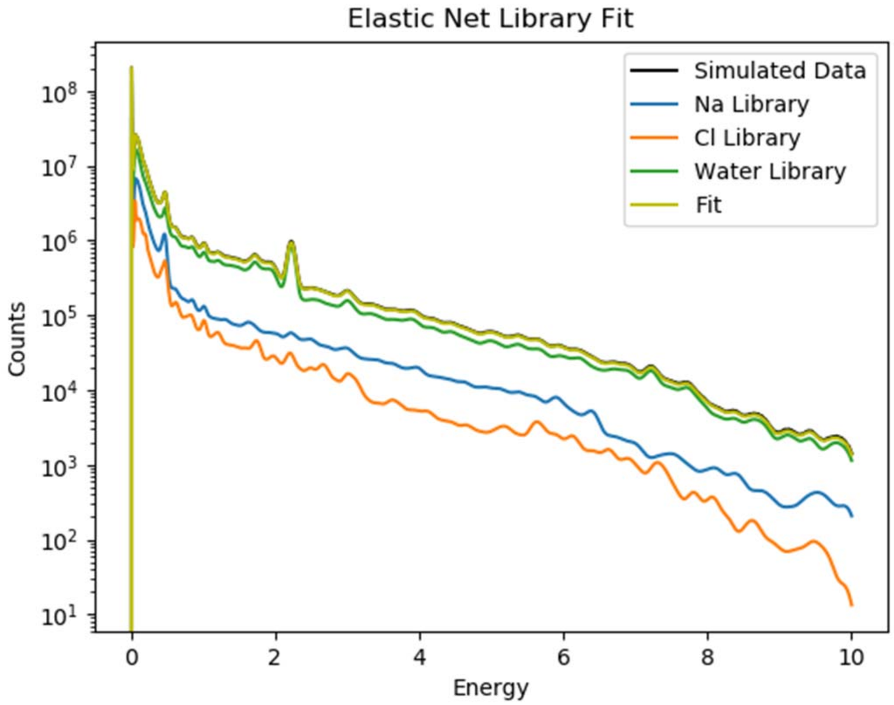
LASSO Simulated Example





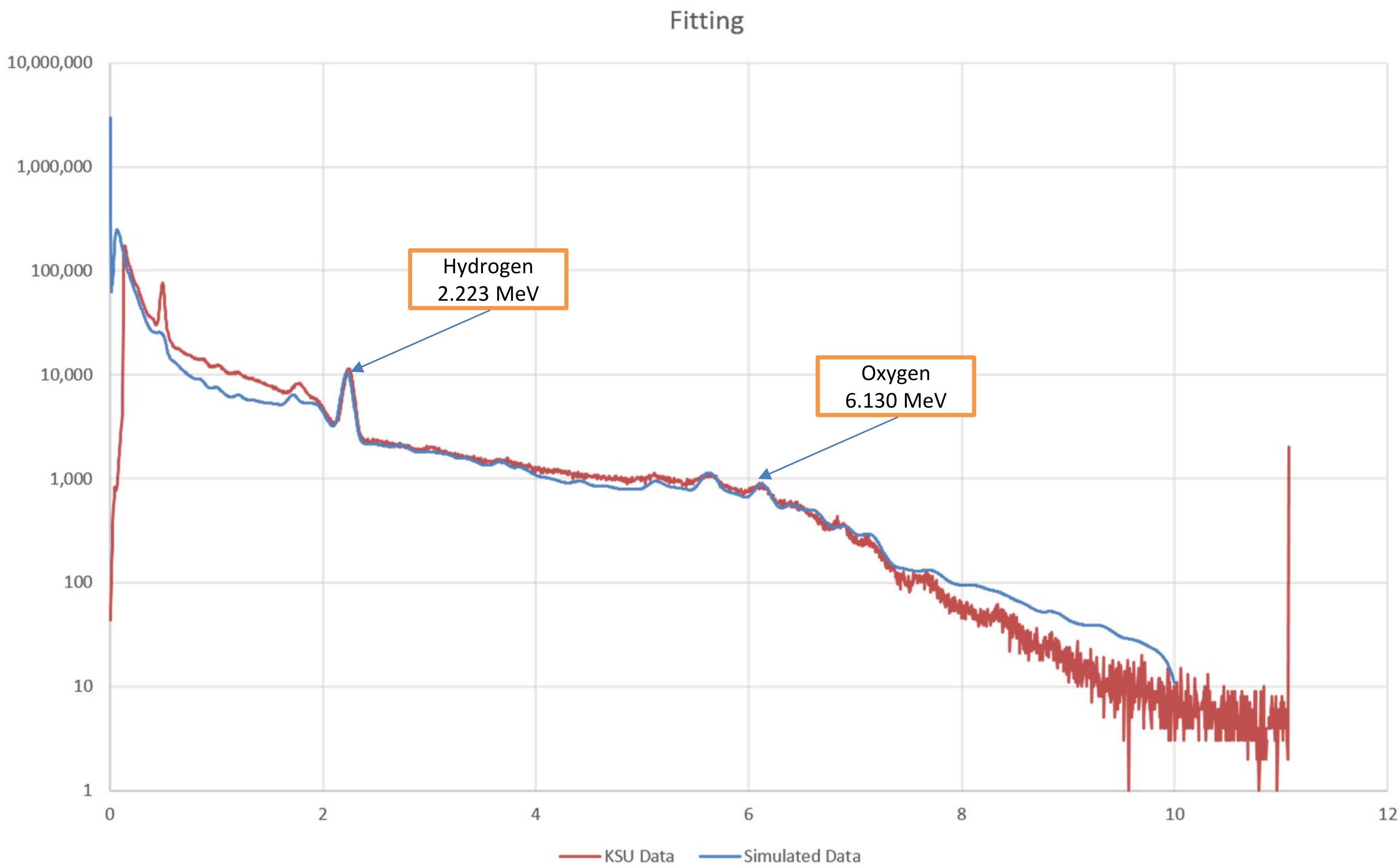
Note: 5 libraries are used. Fe and Cu do not contribute to the total spectrum, are given a 0 contribution and selected out of the final model.

Elastic Net Simulation and Comparison

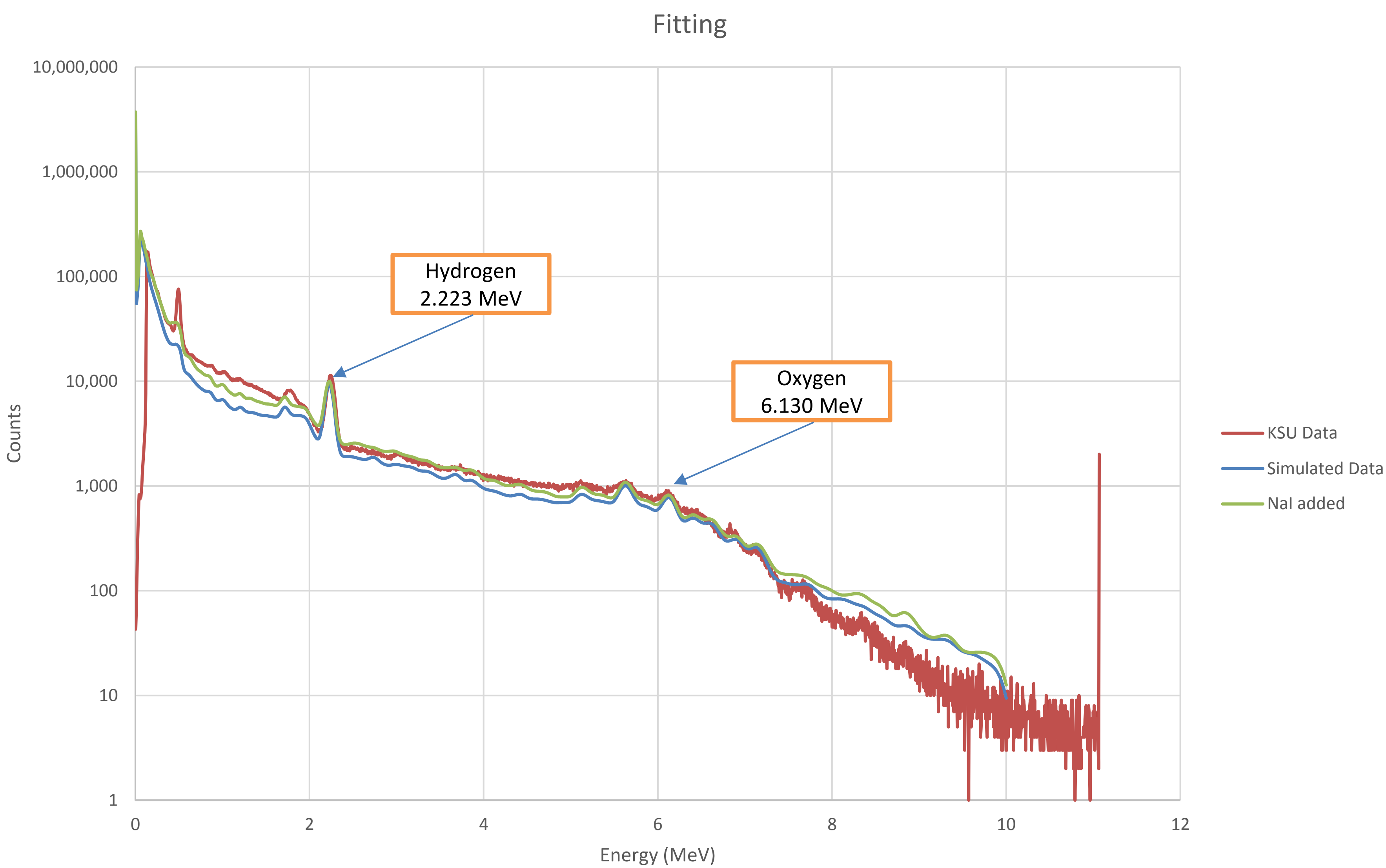


Relative Error		
	Elastic Net	LASSO
Water	5.01%	0.07%
Na	2.95%	1.32%
Cl	29.95%	3.65%

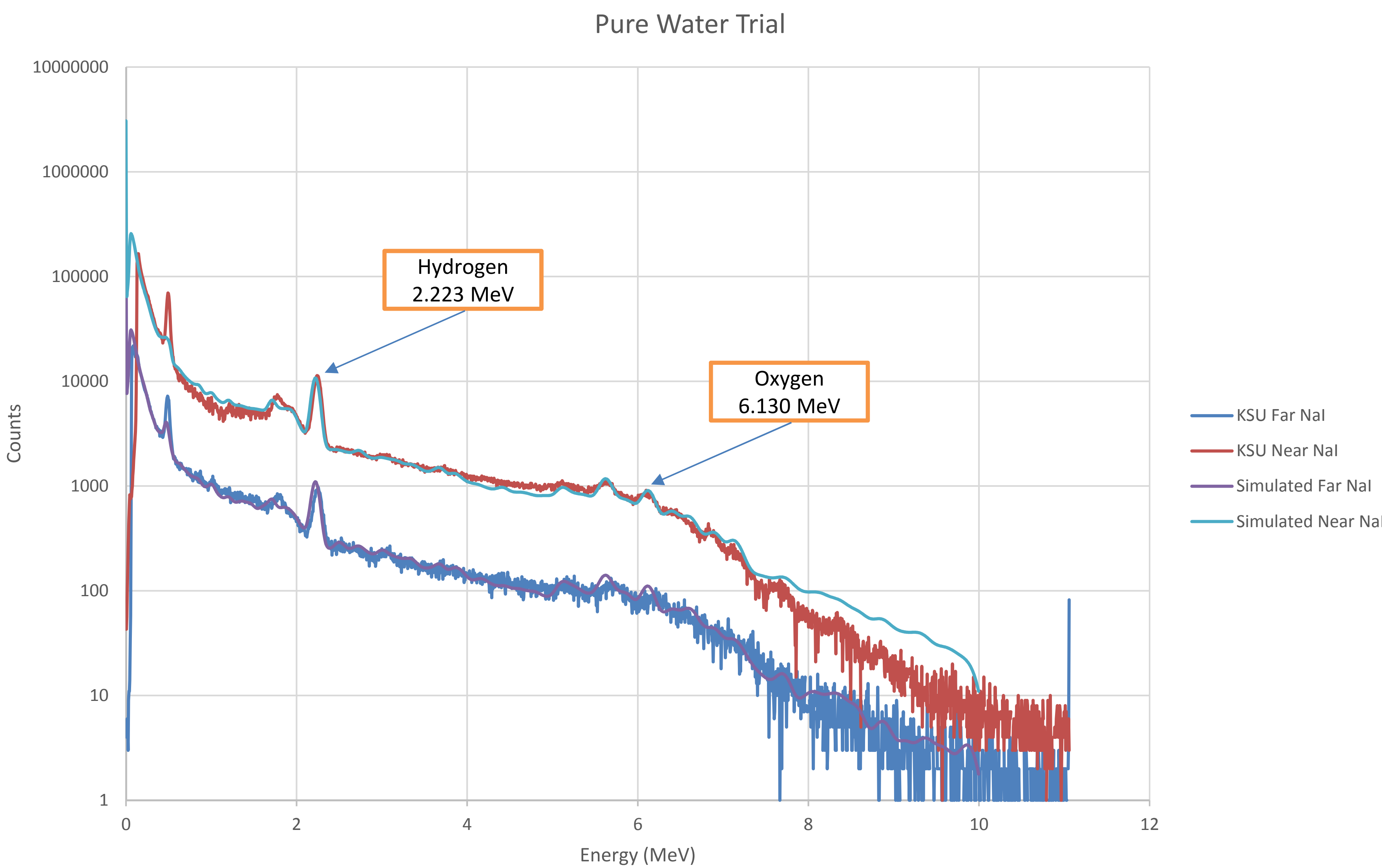
Water – First Results



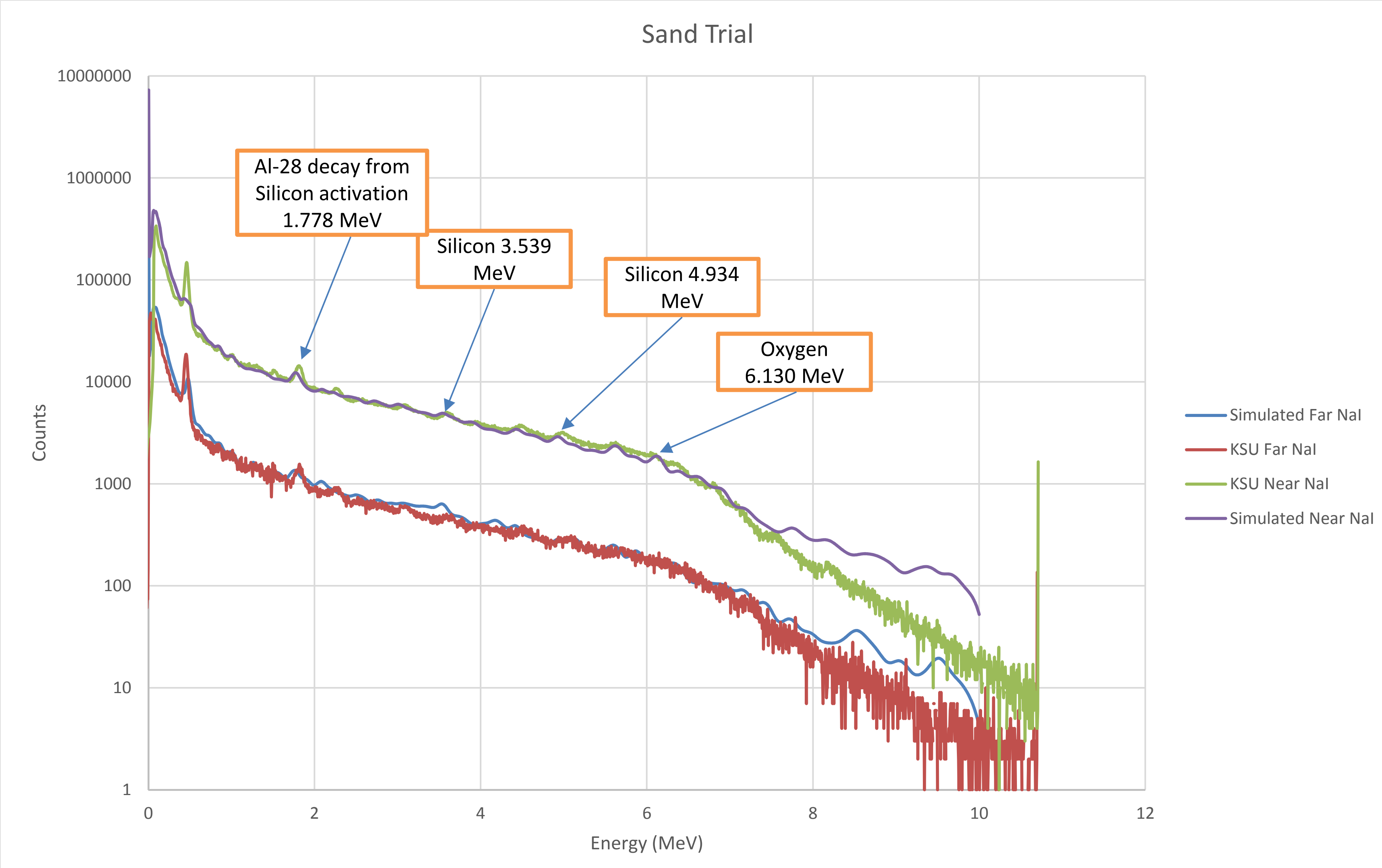
Results With NaI Activation - Water



Water Trial – Background Removed



Sand Trial – Background Removed



Continuing Work/Next Steps

- Incorporate work from Aaron Feinberg and Long Vo
  - Bayesian approach to fit all non-linear components
  - Time dependent digitizer data
- Analyze additional trials run at KSU
  - Limestone
  - Multiple porosities, water content
- Extensive testing of the limitations of LASSO and Elastic Net using simulated radioisotope data
  - High, medium, low counting situations
  - Vary number of radioisotopes
  - Vary number of channels
  - Shielding situations

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Discussion

- Questions?

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