ABSTRACT


In the aftermath of the disasters of September 11th, 2001, new security measures were taken to prevent future attacks. Due to the extreme destructive physical and psychological power of nuclear weapons and radiation dispersal devices, a large effort has been spent in preventing the proliferation of nuclear weapons and materials. Soft targets, such as oil well logging radiochemical sources, have been identified as a commonly used radioactive source that can be replaced by non-active sources such as D-T or D-D pulsed neutron generators.

An experiment at Kansas State University was conducted, using a D-T pulsed neutron generator and test facility to replicate different scenarios commonly found in oil wells. D-T pulsed neutron generators have the ability to generate neutrons at a comparable rate to AmBe and Cf-252 neutron sources. These neutrons then bombard surrounding materials to release gamma rays by inelastic scattering and absorption commonly referred to as prompt gamma neutron activation analysis. D-T pulsed neutron generators produce neutrons at a higher energy than traditional sources, allowing for additional inelastic scattering schemes to be unlocked. Additionally, pulse timing sequences can be manipulated utilizing a digitizer to separate prompt and delayed responses.

This dissertation is devoted to investigating new supervised machine learning algorithms, LASSO and Elastic Net, that are used to automatically perform variable selection and model prediction. MCNP generated libraries are simulated to estimate the detector response using the geometry and material composition of the tool, testing chamber, and surrounding materials and compared to experiments performed at Kansas State University.

During the preliminary work on the oil well logging application, it was discovered that the same techniques could be used as an aid in radioisotope identification devices (RIIDs). Handheld RIIDs are used by first responders and radiation safety personnel to identify radioactive materials found in situ. Simulations of six radioisotopes of similar energy (<1.5 MeV) were generated to investigate how well LASSO and Elastic Net perform in masking and convolution problems in a shielded and unshielded situation.
Preliminary results for each method are promising. Overall, each method accurately selects the correct variables at a rate that should entice oil well logging companies to further investigate integrating these methods into their coding packages to reduce analysis times for their operators. LASSO performs better than Elastic Net in almost every trial conducted during this dissertation and is likely better suited for most radiation detection problems. Elastic Net performs best in applications where the data is highly correlated, and therefore should be considered for any application or situation where the data is correlated.
© Copyright 2019 by Vincent DiNova

All Rights Reserved
Automated Variable Selection of Gamma-Ray Spectra by Utilization of LASSO and Elastic Net Techniques for Use in Nuclear Security Applications

by
Vincent A. DiNova, Jr.

A dissertation submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the requirements for the degree of Doctor of Philosophy

Nuclear Engineering

Raleigh, North Carolina
2019

APPROVED BY:

_______________________________  _______________________________
Dr. Robin Gardner                                                                 Dr. Steven Shannon
Committee Chair                                                                                                           

_______________________________  _______________________________
Dr. Ge Yang                                                    Dr. Ralph Smith
DEDICATION

This dissertation is dedicated to my mother, father, and sister for their constant support and encouragement. To my girlfriend, Stevie, and stepson, Speed, who inspire me to be a Rockstar in every aspect of my life.
BIOGRAPHY

Vincent DiNova was born in Orlando, Florida and traveled the world as the son of a naval officer. After completing high school at Apex High School, he went on to study Nuclear Engineering at NC State University. He completed his B.S. in Nuclear Engineering in 2009 and his M.S. in Nuclear Engineering under the direction of Dr. Robin P. Gardner in 2011. After working 3 years for Bechtel, Vincent returned to NC State University in 2014 to complete his PhD in Nuclear Engineering under the direction of Dr. Robin P. Gardner.
ACKNOWLEDGMENTS

There are so many people who have impacted me on this journey, I hope to capture them all, and I sincerely apologize if I forget any single person. If you read this and think you should have been listed here, believe me that although you are not listed, your impact has been noticed.

The people who have had the largest impact on my life and subsequent work are my family. To my mother and father, Vince and Kay, you have inspired me to be the best man I can be and to push myself to continue to improve every day. To my sister, Kristina, my brother-in-law, Tommy, and my nephew, Jack, my aunts and uncles, Karen, Joe, Nico and Lisa, my memaw and pepaw, and to all my cousins, you have all given me inspiration, examples to follow, and much help when needed. I thank and love you all.

To all my childhood friends who helped shape who I am. I want to especially acknowledge my wonderful friends from Apex High School and their families: Sean Roberts, Matt Baldiga, Kyle Beaulieu, Charlotte Florez, Jill Nee, Nancy Andrews, Darah Willey, Vicki Tucci, Hanna Zombek, Claire Wagner, Gina Winters, Heather Copley, Meredith Caley, Christine Reed, Stephen Mason, and Jenna Ready. All of you helped bring me out of my shell and gain confidence in myself. You and your families became family to me, I think of you all often, and I want you to know I would not have made it here without meeting each of you.

So many people helped me out during my undergraduate degree. To all my professors: Dr. Bourham, Dr. Hawari, Dr. Hanks, Dr. Anistratov, Dr. Doster, and Dr. Turinsky, you all gave me the skills I needed to carry forward to this point. To my classmates, thank you for making life more enjoyable during that period, especially, Aimee Smith, Alison Koeppel, Richard Mongold, Jay Alexander, and Chris Courtenay.

To all of the NC State bowling team, thank you for giving me the best times of my life. I especially want to thank Zack Brown, Jon Scorano, Nick Davis, Brian James, Wes Wheless, Eric Moore, Mike Flitcraft, Rachel Judd, AJ Van Fleet, Kyle Burns, and Craig Nursey. To our coach Irwyn Atkinson, who spent over 30 years coaching the NC State bowling team, you deserve to be immortalized in this work for the contribution you have made to the university and on my life. I thank you for your friendship and mentorship.

To my other bowling team and coworkers, Jimmy Martin, TJ Pocalyko, Bryan Collier, Chris Alexander, Kristin Brown, Dan Moore, Hal Odom, Marge Way, Ben Rose, Barry Pugh, Teddy Ginwright, and Julie Thomas, you are all amazing people, who I try to emulate the best I
can. You have been tremendous friends for so long, and I thank you for all of your help over the years.

To all my peers during graduate school, you have all made these years fun and exciting. I especially want to thank Wes Holmes, Aaron Feinberg, Richard Howard, James Gilman, Adan Calderon, Sean O’brien, Brandon Burns, Andrew Petrarca, Josh Novak, Kyoung Lee, Mario Milev, and Rob Weldon.

To the friends and coworkers I met during my time at Bechtel, for providing me with professional and personal growth, I thank you. I especially want to thank Sarah Fafard, Fotios Raffelis, Hagan Baturay, Dave Dinse, Evan Fredo, Summar Sammons, Hailey Clark, Jimmy and Candi Cole, Stephanie Quinn, Sam Watson, Grant Whitfield, Thomas Ramis, Dan Triplett, and Kenny Hearn.

There are a few people who helped keep me focused during my return to graduate school, Ashley Stancil and her family, Dara O’Sullivan, Rachel Helscher, and Kim Nguyen-Dinh. I thank you for all keeping me on a path that has led me here.

To the NNSA for funding this project and work, and those that helped run the program. I especially want to thank Dr. Mattingly, Dr. Azmy, Stefani Buster, and Russell Villard for helping keep the consortium on track.

To the CNEC students and faculty for their help and support on this project. I especially want to acknowledge Dr. Bill Dunn and Dr. Walter McNeil for setting up the experiment that generated the data used for this project, as well as their students Long Vo, Maria Pinella, Diego Laramore, and Aaron Hellinger.

To Lisa Marshall, for being a great friend and for all the continued excellence you bring to the department and American Nuclear Society.

To my new family, Speed and Stevie, you give me the motivation to be the best I can be. This is as much for you, as any other person. I love you both.

Finally, to my committee, Dr. Shannon, Dr. Yang, and Dr. Smith, you have all been amazing mentors over the years. The impact you have had on my professional and personal growth cannot be measured. Lastly, I want to thank Dr. Gardner for calling me out of the blue in 2014 to get me to return to complete my studies. You have been a tremendous influence on my life for over 12 years and have touched so many lives over the 55+ years at NC State.
There will be more people who will come into my life and have an impact after this moment. This section is for you, I thank you in advance, and look forward to what is to come!
# TABLE OF CONTENTS

**LIST OF TABLES** .................................................................................................................. ix

**LIST OF FIGURES** ................................................................................................................ xi

## Chapter 1: Introduction

1.1 Background ......................................................................................................................... 1
1.2 Benchmarking Tool and Facility ........................................................................................ 3
1.3 Monte Carlo Library Least Squares .................................................................................... 5
1.4 Radioisotope Identification Devices ................................................................................... 6

## Chapter 2: Nuclear Reactions

2.1 Neutron Transport ............................................................................................................... 8
   2.1.1 Neutron Inelastic Scatter (n, n'γ) ............................................................................... 8
   2.1.2 Neutron Capture (n, γ) ............................................................................................... 9
2.2 Photon Transport ............................................................................................................... 10
2.3 Detector Response ............................................................................................................ 13
   2.3.1 Spectral Features ...................................................................................................... 13

## Chapter 3: Machine Learning Enhancements

3.1 Supervised Machine Learning .......................................................................................... 18
   3.1.1 Linear Least Squares ................................................................................................ 18
   3.1.2 Least Absolute Selection and Shrinkage Operator (LASSO) .................................. 19
   3.1.3 Elastic Net ................................................................................................................ 20
   3.1.4 Coordinate Descent Solutions for LASSO and Elastic Net ..................................... 21
      3.1.4.1 LASSO Single Variable Case ....................................................................... 22
      3.1.4.2 Coordinate Descent for LASSO ................................................................... 23
      3.1.4.3 Coordinate Descent for Elastic Net .............................................................. 25
   3.1.5 Cross Validation....................................................................................................... 27

## Chapter 4: Kansas State Experiment

4.1 Data Collection ................................................................................................................. 29
   4.1.1 Kansas State Experimental Data .............................................................................. 29
   4.1.2 Simulated Data ......................................................................................................... 30
   4.1.3 Simulated Example ................................................................................................. 30
4.2 Methods and Improvements .............................................................................................. 34
   4.2.1 Full Procedure .......................................................................................................... 34
   4.2.2 Early Lessons Learned............................................................................................. 35
4.3 Kansas State Experimental Results ................................................................................... 38
   4.3.1 Water Trial ............................................................................................................... 39
   4.3.2 Sand Trial ................................................................................................................ 50
   4.3.3 Sand with Water Trial ............................................................................................ 61
   4.3.4 Limestone Trial ....................................................................................................... 72
   4.3.5 Limestone with Water Trial .................................................................................... 83
4.4 Discussion ......................................................................................................................... 94
Chapter 5: Radioisotope Identification Device Algorithm ................................................................. 95
  5.1 Data Collection ......................................................................................................................... 95
  5.2 Masking Without Shielding ..................................................................................................... 96
  5.3 Convolution Without Shielding ............................................................................................. 101
  5.4 Masking with Shielding .......................................................................................................... 105
  5.5 Convolution with Shielding .................................................................................................. 109

Chapter 6: Discussion and Conclusions ............................................................................................. 114

References ........................................................................................................................................ 116

Appendices .................................................................................................................................... 119

Appendix A: MCNP Sample Deck – KSU Application ................................................................. 120

Appendix B: LASSO Code Sample .............................................................................................. 125

Appendix C: Elastic Net Code Sample ......................................................................................... 128
LIST OF TABLES

Table 1-1: NAS findings ........................................................................................................... 1
Table 2-1: Non-elastic scattering reactions and threshold energies........................................... 9
Table 3-1: Full LASSO Coordinate Descent Algorithm.......................................................... 25
Table 3-2: Full Elastic Net Coordinate Descent Algorithm..................................................... 27
Table 4-1: Relative error of the two methods ......................................................................... 34
Table 4-2: Optimal normalization parameters for water trial ................................................. 47
Table 4-3: Linear coefficients and error for water near detector ............................................. 49
Table 4-4: Linear coefficients and error for water far detector ............................................... 50
Table 4-5: Optimal normalization parameters for sand trial.................................................... 59
Table 4-6: Linear coefficients and error for sand near detector ............................................. 61
Table 4-7: Linear coefficients and error for sand far detector ................................................... 61
Table 4-8: Optimal normalization parameters for sand and water trial .................................. 70
Table 4-9: Linear coefficients and error for sand and water near detector ............................. 72
Table 4-10: Linear coefficients and error for sand and water far detector .............................. 72
Table 4-11: Optimal normalization parameters for limestone trial ....................................... 81
Table 4-12: Linear coefficients and error for limestone near detector ................................... 83
Table 4-13: Linear coefficients and error for limestone far detector ........................................ 83
Table 4-14: Optimal normalization parameters for limestone and water trial ....................... 92
Table 4-15: Linear coefficients and error for limestone and water near detector ................... 94
Table 4-16: Linear coefficients and error for limestone and water far detector ..................... 94
Table 5-1: Masking coefficients and total count .................................................................... 97
Table 5-2: Masking trial prediction accuracy for LASSO and Elastic Net with varying count rates .................................................................................................................. 100
Table 5-3: Convolution coefficients and total counts ................................................................. 101

Table 5-4: Convolution trial prediction accuracy for LASSO and Elastic Net with varying count rates ................................................................. 105

Table 5-5: Masking with shielding coefficients and total counts ........................................... 106

Table 5-6: Masking with shielding trial prediction accuracy for LASSO and Elastic Net with varying count rates ................................................. 109

Table 5-7: Convolution with shielding coefficients and total counts .................................... 110

Table 5-8: Convolution with shielding trial prediction accuracy for LASSO and Elastic Net with varying count rates ........................................... 113
LIST OF FIGURES

Figure 1-1: Prompt and delayed gamma ray emission process .................................................... 2
Figure 1-2: KSU benchmarking tool ........................................................................................... 3
Figure 1-3: Data acquisition scheme............................................................................................ 3
Figure 1-4: KSU design facility ................................................................................................... 4
Figure 1-5: Test chamber ............................................................................................................. 4
Figure 1-6: a. Open borehole tube, b. Capped borehole tube ....................................................... 5
Figure 2-1: Depiction of the Photoelectric Effect ...................................................................... 10
Figure 2-2: Depiction of the Compton Scattering process ......................................................... 11
Figure 2-3: Illustration of the Compton edge and continuum .................................................... 11
Figure 2-4: Depiction of interaction of gamma-rays with a detector medium and
their resultant spectra .................................................................................................................. 12
Figure 2-5: Energy dependence of photon interactions in NaI .................................................. 13
Figure 2-6: Infinite resolution detector response .......................................................................... 14
Figure 3-1: Soft-thresholding function ....................................................................................... 22
Figure 3-2: Holdout method for test-train split .......................................................................... 28
Figure 3-3: Cross validation holdout ........................................................................................... 28
Figure 4-1: F8 tally simulated response and Gaussian broadened detector response ............ 30
Figure 4-2: Cross validation normalization parameter selection for LASSO ......................... 31
Figure 4-3: LASSO model selection coefficients by changing normalization parameter .......... 31
Figure 4-4: LASSO salt water simulation fit ............................................................................. 32
Figure 4-5: Cross validation normalization parameter selection for Elastic Net ....................... 32
Figure 4-6: Elastic Net model selection by changing normalization parameter ........................ 33
Figure 4-7: Elastic Net salt water simulation fit ........................................................................ 33
Figure 4-8: Full procedure........................................................................................................ 35

Figure 4-9: Pure water first fit............................................................................................ 36

Figure 4-10: Pure water fit with NaI activation libraries added .......................................... 36

Figure 4-11: Firing sequence and measured response......................................................... 37

Figure 4-12: Time dependent format distributed by Kansas State University...................... 38

Figure 4-13: Cross validation normalization parameter selection for the
LASSO near detector water trial ......................................................................................... 39

Figure 4-14: LASSO model selection coefficients by changing the normalization
parameter for the near detector water trial ..................................................................... 40

Figure 4-15: LASSO fit for the near detector water trial..................................................... 40

Figure 4-16: LASSO full fit for the near detector water trial............................................... 41

Figure 4-17: Cross validation normalization parameter selection for the
Elastic Net near detector water trial .................................................................................. 41

Figure 4-18: Elastic Net model selection coefficients by changing the normalization
parameter for the near detector water trial ..................................................................... 42

Figure 4-19: Elastic Net fit for the near detector water trial............................................... 42

Figure 4-20: Elastic Net full fit for the near detector water trial......................................... 43

Figure 4-21: Cross validation normalization parameter selection for the
LASSO far detector water trial ......................................................................................... 43

Figure 4-22: LASSO model selection coefficients by changing the normalization
parameter for the far detector water trial ........................................................................ 44

Figure 4-23: LASSO fit for the far detector water trial ....................................................... 44

Figure 4-24: LASSO full fit for the far detector water trial.................................................. 45

Figure 4-25: Cross validation normalization parameter selection for the
Elastic Net far detector water trial .................................................................................... 45

Figure 4-26: Elastic Net model selection coefficients by changing the normalization
parameter for the far detector water trial ........................................................................ 46
Figure 4-27: Elastic Net fit for the far detector water trial ................................................................. 46
Figure 4-28: Elastic Net full fit for the far detector water trial ............................................................... 47
Figure 4-29: Linear least squares fit and residual for the near detector water trial ............................ 48
Figure 4-30: Linear least squares fit and residual for the far detector water trial ............................... 48
Figure 4-31: Linear least squares fit for near and far detector water trials ........................................ 49
Figure 4-32: Cross validation normalization parameter selection for the LASSO near detector sand trial ................................................................................................................................. 51
Figure 4-33: LASSO model selection coefficients by changing the normalization parameter for the near detector sand trial .................................................................................................................. 51
Figure 4-34: LASSO fit for the near detector sand trial .......................................................... 52
Figure 4-35: LASSO full fit for the near detector sand trial ............................................................ 52
Figure 4-36: Cross validation normalization parameter selection for the Elastic Net near detector sand trial ................................................................................................................................. 53
Figure 4-37: Elastic Net model selection coefficients by changing the normalization parameter for the near detector sand trial .................................................................................................................. 53
Figure 4-38: Elastic Net fit for the near detector sand trial .......................................................... 54
Figure 4-39: Elastic Net full fit for the near detector sand trial ............................................................ 54
Figure 4-40: Cross validation normalization parameter selection for the LASSO far detector sand trial ................................................................................................................................. 55
Figure 4-41: LASSO model selection coefficients by changing the normalization parameter for the far detector sand trial .................................................................................................................. 55
Figure 4-42: LASSO fit for the far detector sand trial .......................................................... 56
Figure 4-43: LASSO full fit for the far detector sand trial ............................................................ 56
Figure 4-44: Cross validation normalization parameter selection for the Elastic Net far detector sand trial ................................................................................................................................. 57
Figure 4-45: Elastic Net model selection coefficients by changing the normalization parameter for the far detector sand trial .................................................................................................................. 57
Figure 4-46: Elastic Net fit for the far detector sand trial ........................................................... 58

Figure 4-47: Elastic Net full fit for the far detector sand trial .................................................... 58

Figure 4-48: Linear least squares fit and residual for the near detector sand trial ...................... 59

Figure 4-49: Linear least squares fit and residual for the far detector sand trial ...................... 60

Figure 4-50: Linear least squares fit for near and far detector sand trials ............................. 60

Figure 4-51: Cross validation normalization parameter selection for the
LASSO near detector sand and water trial ............................................................................. 62

Figure 4-52: LASSO model selection coefficients by changing the normalization
parameter for the near detector sand and water trial ......................................................... 62

Figure 4-53: LASSO fit for the near detector sand and water trial ........................................... 63

Figure 4-54: LASSO full fit for the near detector sand and water trial ................................. 63

Figure 4-55: Cross validation normalization parameter selection for the
Elastic Net near detector sand and water trial ..................................................................... 64

Figure 4-56: Elastic Net model selection coefficients by changing the normalization
parameter for the near detector sand and water trial ......................................................... 64

Figure 4-57: Elastic Net fit for the near detector sand and water trial ..................................... 65

Figure 4-58: Elastic Net full fit for the near detector sand and water trial ............................. 65

Figure 4-59: Cross validation normalization parameter selection for the
LASSO far detector sand and water trial ............................................................................. 66

Figure 4-60: LASSO model selection coefficients by changing the normalization
parameter for the far detector sand and water trial ......................................................... 66

Figure 4-61: LASSO fit for the far detector sand and water trial ........................................... 67

Figure 4-62: LASSO full fit for the far detector sand and water trial ..................................... 67

Figure 4-63: Cross validation normalization parameter selection for the
Elastic Net far detector sand and water trial ..................................................................... 68

Figure 4-64: Elastic Net model selection coefficients by changing the normalization
parameter for the far detector sand and water trial ......................................................... 68
Figure 4-65: Elastic Net fit for the far detector sand and water trial ........................................... 69
Figure 4-66: Elastic Net full fit for the far detector sand and water trial................................. 69
Figure 4-67: Linear least squares fit and residual for the near detector sand and water trial .... 70
Figure 4-68: Linear least squares fit and residual for the far detector sand and water trial....... 71
Figure 4-69: Linear least squares fit for near and far detector sand and water trials ............ 72
Figure 4-70: Cross validation normalization parameter selection for the LASSO near detector limestone trial .......................................................... 73
Figure 4-71: LASSO model selection coefficients by changing the normalization parameter for the near detector limestone trial .................................................. 73
Figure 4-72: LASSO fit for the near detector limestone trial ..................................................... 74
Figure 4-73: LASSO full fit for the near detector limestone trial ............................................. 74
Figure 4-74: Cross validation normalization parameter selection for the Elastic Net near detector limestone trial ................................................................. 75
Figure 4-75: Elastic Net model selection coefficients by changing the normalization parameter for the near detector limestone trial ............................................... 75
Figure 4-76: Elastic Net fit for the near detector limestone trial ................................................. 76
Figure 4-77: Elastic Net full fit for the near detector limestone trial ........................................... 76
Figure 4-78: Cross validation normalization parameter selection for the LASSO far detector limestone trial ................................................................. 77
Figure 4-79: LASSO model selection coefficients by changing the normalization parameter for the far detector limestone trial ............................................... 77
Figure 4-80: LASSO fit for the far detector limestone trial ....................................................... 78
Figure 4-81: LASSO full fit for the far detector limestone trial ................................................... 78
Figure 4-82: Cross validation normalization parameter selection for the Elastic Net far detector limestone trial ................................................................. 79
Figure 4-83: Elastic Net model selection coefficients by changing the normalization parameter for the far detector limestone trial ............................................... 79
Figure 4-84: Elastic Net fit for the far detector limestone trial.................................80
Figure 4-85: Elastic Net full fit for the far detector limestone trial..............................80
Figure 4-86: Linear least squares fit and residual for the near detector limestone trial.........81
Figure 4-87: Linear least squares fit and residual for the far detector limestone trial........28
Figure 4-88: Linear least squares fit for near and far detector limestone trials.................82
Figure 4-89: Cross validation normalization parameter selection for the
LASSO near detector limestone and water trial..................................................84
Figure 4-90: LASSO model selection coefficients by changing the normalization
parameter for the near detector limestone and water trial....................................84
Figure 4-91: LASSO fit for the near detector limestone and water trial .........................85
Figure 4-92: LASSO full fit for the near detector limestone and water trial......................85
Figure 4-93: Cross validation normalization parameter selection for the
Elastic Net near detector limestone and water trial............................................86
Figure 4-94: Elastic Net model selection coefficients by changing the normalization
parameter for the near detector limestone and water trial....................................86
Figure 4-95: Elastic Net fit for the near detector limestone and water trial .....................87
Figure 4-96: Elastic Net full fit for the near detector limestone and water trial..................87
Figure 4-97: Cross validation normalization parameter selection for the
LASSO far detector limestone and water trial....................................................88
Figure 4-98: LASSO model selection coefficients by changing the normalization
parameter for the far detector limestone and water trial....................................88
Figure 4-99: LASSO fit for the far detector limestone and water trial............................89
Figure 4-100: LASSO full fit for the far detector limestone and water trial.....................89
Figure 4-101: Cross validation normalization parameter selection for the
Elastic Net far detector limestone and water trial..............................................90
Figure 4-102: Elastic Net model selection coefficients by changing the normalization
parameter for the far detector limestone and water trial....................................90
Figure 4-103: Elastic Net fit for the far detector limestone and water trial ................................ 91

Figure 4-104: Elastic Net full fit for the far detector limestone and water trial ................. 91

Figure 4-105: Linear least squares fit and residual for the near detector limestone and water trial ................................................................. 92

Figure 4-106: Linear least squares fit and residual for the far detector limestone and water trial ................................................................. 93

Figure 4-107: Linear least squares fit for near and far detector limestone and water trials ...... 93

Figure 5-1: Vised depiction of detector geometry ................................................................. 96

Figure 5-2: MCNP generated radioisotope libraries .............................................................. 96

Figure 5-3: LASSO masking low count rate fit ..................................................................... 97

Figure 5-4: Elastic Net masking low count rate fit ............................................................... 98

Figure 5-5: LASSO masking medium count rate fit ............................................................. 98

Figure 5-6: Elastic Net masking medium count rate fit ....................................................... 99

Figure 5-7: LASSO masking high count rate fit ................................................................... 99

Figure 5-8: Elastic Net masking high count rate fit ............................................................ 100

Figure 5-9: LASSO convolution low count rate fit .............................................................. 102

Figure 5-10: Elastic Net convolution low count rate fit ....................................................... 102

Figure 5-11: LASSO convolution medium count rate fit .................................................... 103

Figure 5-12: Elastic Net convolution medium count rate fit ............................................. 103

Figure 5-13: LASSO convolution high count rate fit ......................................................... 104

Figure 5-14: Elastic Net convolution high count rate fit .................................................... 104

Figure 5-15: LASSO masking with shielding low count rate fit ....................................... 106

Figure 5-16: Elastic Net masking with shielding low count rate fit .................................. 107

Figure 5-17: LASSO masking medium count rate fit ......................................................... 107
Figure 5-18: Elastic Net masking with shielding medium count rate fit ........................................ 108
Figure 5-19: LASSO masking with shielding high count rate fit .................................................. 108
Figure 5-20: Elastic Net masking with shielding high count rate fit ........................................ 109
Figure 5-21: LASSO convolution with shielding low count rate fit ........................................... 110
Figure 5-22: Elastic Net convolution with shielding low count rate fit ..................................... 111
Figure 5-23: LASSO convolution with shielding medium count rate fit .................................. 111
Figure 5-24: Elastic Net convolution with shielding medium count rate fit .............................. 112
Figure 5-25: LASSO convolution with shielding high count rate fit ........................................ 112
Figure 5-26: Elastic Net convolution with shielding high count rate fit ................................... 113
CHAPTER 1

Introduction

1.1 Background

Shortly after the tragedies of September 11, 2001, the National Academies of Science commissioned a study on the dangers of long-lived radioisotope sources. The study concluded that there exist several commonly used sources that could potentially be used as a dirty bomb or terror weapon (Table 1-1). The Consortium for Nonproliferation Enabling Capabilities (CNEC) was funded in 2014 to research innovative ways to address nuclear security problems including finding suitable replacements for dangerous radiological sources.

<table>
<thead>
<tr>
<th>Radionuclide</th>
<th>Half-life (yr)</th>
<th>Particles-Energies (MeV)</th>
<th>Principal Applications</th>
<th>US Inventory (Ci)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cs-137</td>
<td>30.17</td>
<td>β-0.518 max; β-1.18 max; γ-0.662</td>
<td>Industrial gauging, Irradiators, Well logging</td>
<td>2,800,000</td>
</tr>
<tr>
<td>Co-60</td>
<td>5.27</td>
<td>γ-1.173; γ-1.333</td>
<td>Sterilization, Irradiators, Teletherapy</td>
<td>198,000,000</td>
</tr>
<tr>
<td>Am-241</td>
<td>432.2</td>
<td>α-5.64; γ-0.060</td>
<td>Well logging, Gauging</td>
<td>6,482</td>
</tr>
<tr>
<td>Pu-238</td>
<td>87.7</td>
<td>α-5.59; γ-0.043</td>
<td>RTGs</td>
<td>937</td>
</tr>
<tr>
<td>Sr-90</td>
<td>28.9</td>
<td>β-0.546 max</td>
<td>RTGs</td>
<td>1,730,000</td>
</tr>
<tr>
<td>Se-75</td>
<td>119.8 d</td>
<td>γ-0.28 (ave), 0.8 max</td>
<td>Radiography</td>
<td>261</td>
</tr>
<tr>
<td>Ir-192</td>
<td>74 d</td>
<td>β-1.46 max; γ-0.38 ave, 1.378 max</td>
<td>Radiography</td>
<td>146,922</td>
</tr>
<tr>
<td>Cf-252</td>
<td>2.645</td>
<td>α-6.22; n-2 ave; γ-various; fission products</td>
<td>Well logging Research</td>
<td>7</td>
</tr>
</tbody>
</table>

Devices used in the oil well logging industry were identified as a major point of interest as they utilize high activity Cs-137 and AmBe sources for density, porosity, and elemental composition measurements. A testing facility and benchmarking tool were designed and built at Kansas State University to test the viability of replacing traditional active sources with a D-T Pulsed Neutron Generator (PNG). A PNG operates by receiving a signal to initialize a pulse.
firing sequence that propels Deuterons and Tritons on a collision path releasing 14.1 MeV neutrons. These high-energy neutrons are used as an alternative to AmBe neutrons in a traditional prompt gamma neutron activation analysis (PGNAA) application. PGNAA is a nondestructive method that relies on (n, γ) neutron capture, and (n, n’γ) neutron inelastic scattering reactions to produce gamma photons, each having distinct characteristics of the target nuclei. Using a near and far NaI scintillator detector, each spectral detector response can be analyzed for elemental composition.

PGNAA suffers from a low signal to noise ratio caused by the delayed activation of nuclei or neutron activation analysis (NAA). Neutron activation analysis utilizes the delayed gamma rays from radioactive daughters, while PGNAA exploits the prompt gamma rays (Fig. 1-1). The neutron cross sections for both prompt and delayed reactions compete and create a mixed signal that is often difficult to process. Additional sources of interference include:

1) γ rays produced by the PNG
2) γ rays from activation inside the detector medium (Gardner, 2000)
3) γ rays from background sources
4) γ rays produced by the activation of construction materials in the benchmarking tool.

The PNG offers a unique solution to this problem by exploiting the pulsing time responses with a digitizer allowing the prompt and delayed responses to be extracted and separated. This critical step allows for supervised machine learning variable selection techniques such as LASSO and Elastic Net to be applied to the prompt and delayed responses, offering an on-line analysis in a changing environment with improved capabilities over traditional linear least squares methods.
1.2 Benchmarking tool and facility

The benchmarking tool and design facility were designed and constructed at Kansas State University. The tool consists of near and far gamma and neutron detectors separated from a D-T PNG source by a 2” lead divider (Fig. 1-2). A CAEN 5730 digitizer acts to both send the pulse firing sequence to the PNG and to collect the responses from the gamma and neutron detectors (Fig. 1-3).

![KSU benchmarking tool](image1)

The design facility (Fig. 1-4) is located at King Hall Annex at Kansas State University. Special accelerator enabling systems were required to gain approval from the Kansas Safety Board to prevent inadvertent neutron production and entries into the facility. These safeguards include audio and video surveillance, controlled access points, intercommunication systems, warning lights, and detailed operating procedures to minimize unnecessary dosage to bystanders.
The test chamber (Figs. 1-5, 1-6) is 6’8” high by 6’6” wide and 8’ deep with a total volume of roughly 2,500 gallons. These dimensions ensure that when fully filled with water, the test chamber presents an effectively infinite medium to the 14.1 MeV neutrons. During the data collection process, the benchmarking tool is loaded into the borehole tube and enclosed by a cap. Borated polyethylene (green material) has been fitted both inside and outside the test chamber to reduce neutron escape and dosage.
1.3 Monte Carlo Library Least Squares

In order to quantitatively analyze measured PGNAA γ spectra, Monte Carlo Library Least Squares (MCLLS) has been shown to be an effective method over single peak analysis (Gardner, 1997). MCLLS requires extremely accurate forward model simulations to represent the expected pulse-height spectrum obtained with a PGNAA system with a known geometry and compositional makeup. Previous studies have demonstrated the effectiveness on bulk coal (Shyu et al., 1988, 1998) and PGNAA applications (Han, 2005 and Hou, 2017). The MCLLS approach consists of:

1) Generating pulse-height spectra with MCNP or similar coding packages using assumed or known geometry and compositions.
2) Utilizing each prompt γ-ray pulse-height spectrum as a library input variable for model selection.
3) Adjusting all non-linear parameters between simulated and experimental response to treat the problem as a sum of linear responses.
4) Perform a linear library least-squares (LLS) analysis.

Assuming all non-linear physical components are correctly adjusted, the library least-squares method treats an unknown sample as the sum of the products of an elemental amount with the library spectrum of each element for each channel as given by equation 1.1.

\[ y_i = \sum_{j=1}^{m} a_j x_{ij} + e_j \quad i = 1,2,3,...,n \]
Where,

- $y_i$ is the counts per channel $i$ of an unknown spectrum
- $a_j$ are linear coefficients for each element $j$
- $x_{ij}$ are the library spectra, or counts in channel $i$ of element $j$
- $e_i$ is random error in counts in channel $i$

Equation 1.1 is solved for $x_j$ by minimizing the reduced Chi-Square $\chi^2_0$ given by equation 1.2.

$$\chi_0^2 = \sum_{i=1}^{n} \frac{e_i^2}{(n-m)\sigma_i^2}$$

Where,

- $(n-m)$ is the number of degrees of freedom
- $e_i$ is random error in counts in channel $i$
- $\sigma_i^2$ is the variance of the random error in counts in each channel $i$

### 1.4 Radioisotope Identification Devices

During this investigation using LASSO and Elastic Net variable selection techniques on oil well logging devices, radioisotope identification devices (RIIDs) were targeted as another application that could be improved by the use of these algorithms. RIIDs are handheld instruments designed to identify radioactive materials by their emitted gamma ray energies. RIID algorithm development is necessary to ensure that potential threats are correctly identified by field agents and first responders. A study from 2003 concluded that only 30%-50% of medical, industrial, NORM, and threat isotopes were correctly identified (Blackadar et al).

RIID algorithms measure similarities between measured characteristics of test spectrum and reference spectra, whether experimental or simulated. Many challenges emerge as a result of variations that occur naturally (Burr and Hamada, 2009) including:

- Absorbers can attenuate counts differentially with respect to energy, causing distorted pulse height distributions.
- Voltage calibrations can be nonlinear, and electronic gain shift effects can be nonlinear and unstable over time due to environmental effects.
- Procedural protocols can complicate the required measurements. Temperature and spatial factors can impact the calibration and collection time necessary to collect accurate measurements.
- There can be hundreds of isotopes in the isotope library, each with numerous example spectra.
- Detector dead time and pulse pile up can distort the test spectra.

Due to inadequate RIID algorithm performance, the U.S. Department of Energy (DOE) requires trained spectroscopists to be on call to resolve alarms as rapidly as possible. It was identified that human experts outperform even the best RIID algorithms, leading to the study of supervised machine learning techniques established by experts to help address these shortcomings.
CHAPTER 2

Nuclear Reactions

Prompt gamma-ray neutron activation analysis (PGNAA) is a nondestructive, near real time technique used for bulk material identifications. PGNAA relies on neutron inelastic scatter and capture reactions to produce characteristic γ-rays used to identify minute amounts of elements in a bulk sample. Due to low cross sections for these reactions, background sources from natural radiation, activation of the NaI detector, and γ-rays from the decay of the neutron source a low signal to noise ratio (SNR) is common.

2.1 Neutron Transport

There are a number of different mechanisms by which neutrons can interact with nuclei. For the prompt gamma neutron activation analysis application, only two are considered.

2.1.1 Neutron Inelastic Scatter (n, n’γ)

Neutron inelastic scatter involves an incoming neutron colliding with a target nucleus and exiting with less energy and at a different angle than it entered. The energy deposited on the target nucleus causes it to reach an excited state and rapidly releases a γ-ray to return to its normal energy state represented in equation 2.1 as follows:

\[ _1^0n + _2^4X \rightarrow _1^0n' + _2^4X^* \]  

(2.1)

The inelastic scattering reaction requires an incoming neutron to have enough energy to break the threshold energy derived from the Q value formula shown in equation 2.2.

\[ T_n \geq E_{L1} \frac{A + 1}{A} \]  

(2.2)
Where,

- $T_n$ is the kinetic energy of the incident neutron
- $E_{l1}$ is the energy of the target nucleus’ first excited level
- $A$ is the atomic number of the target nucleus

The PNG is advantageous for this decay scheme, as the 14.1 MeV neutrons allow a greater number of isotopes to undergo inelastic scattering and unlock higher energy states. Table 2-1 (Kim et al. 2006) below lists some common inelastic scatter threshold energies and cross sections.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Gamma Ray Energy, keV</th>
<th>Threshold, MeV</th>
<th>Peak Cross Section, mb</th>
<th>Energy of Peak, MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}\text{C}(n,\gamma)^{12}\text{C}$</td>
<td>4438.0</td>
<td>4.8</td>
<td>450.0</td>
<td>8.1</td>
</tr>
<tr>
<td>$^{16}\text{O}(n,\gamma)^{16}\text{O}$</td>
<td>6128.6</td>
<td>6.6</td>
<td>265.0</td>
<td>7.5–9.0</td>
</tr>
<tr>
<td>$^{16}\text{O}(n,p)^{16}\text{N}$</td>
<td>6128.6</td>
<td>10.6</td>
<td>50.0</td>
<td>11.5</td>
</tr>
<tr>
<td>$^{16}\text{O}(n,\gamma)^{16}\text{N}$</td>
<td>5269.2</td>
<td>16.5</td>
<td>40.0</td>
<td>27.5</td>
</tr>
<tr>
<td>$^{16}\text{O}(n,\alpha)^{12}\text{C}$</td>
<td>4438.0</td>
<td>12.3</td>
<td>130.0</td>
<td>19.0</td>
</tr>
<tr>
<td>$^{24}\text{Mg}(n,\gamma)^{27}\text{Mg}$</td>
<td>1368.6</td>
<td>1.4</td>
<td>600.0</td>
<td>2.5–6.0</td>
</tr>
<tr>
<td>$^{27}\text{Al}(n,\gamma)^{30}\text{Al}$</td>
<td>1014.4</td>
<td>1.1</td>
<td>220.0</td>
<td>2.5–6.7</td>
</tr>
<tr>
<td>$^{27}\text{Al}(n,\alpha)^{24}\text{Mg}$</td>
<td>221.1</td>
<td>2.25</td>
<td>210.0</td>
<td>7.0–9.5</td>
</tr>
<tr>
<td>$^{28}\text{Si}(n,\gamma)^{31}\text{Si}$</td>
<td>1779.9</td>
<td>1.8</td>
<td>770.0</td>
<td>4.5–6.0</td>
</tr>
<tr>
<td>$^{32}\text{S}(n,\gamma)^{35}\text{S}$</td>
<td>2230.1</td>
<td>2.3</td>
<td>440.0</td>
<td>6.7–10.0</td>
</tr>
<tr>
<td>$^{40}\text{Ar}(n,\gamma)^{43}\text{Ar}$</td>
<td>1460.8</td>
<td>1.5</td>
<td>800.0</td>
<td>3.0–10.0</td>
</tr>
<tr>
<td>$^{40}\text{Ar}(n,\alpha)^{37}\text{Cl}$</td>
<td>1460.8</td>
<td>8.0</td>
<td>20.0</td>
<td>14.5</td>
</tr>
<tr>
<td>$^{40}\text{Ca}(n,\alpha)^{37}\text{Ca}$</td>
<td>3736.5</td>
<td>3.8</td>
<td>130.0</td>
<td>7.0</td>
</tr>
<tr>
<td>$^{56}\text{Fe}(n,\gamma)^{59}\text{Fe}$</td>
<td>846.8</td>
<td>0.9</td>
<td>1150.0</td>
<td>6.0</td>
</tr>
<tr>
<td>$^{56}\text{Fe}(n,\gamma)^{61}\text{Cu}$</td>
<td>1238.3</td>
<td>2.1</td>
<td>475.0</td>
<td>16.5</td>
</tr>
</tbody>
</table>

**2.1.2 Neutron Capture (n, γ)**

Neutron capture, also denoted as (n, γ), can occur over a wide range of energies and has the highest probability at thermal energies. The (n, γ) reaction begins when a neutron interacts with a target nucleus and is absorbed. The newly formed nucleus is placed in an excited state, and in order to form a new ground state, at least one γ photon is emitted as shown in eq. 2.3 below.

$$ ^1_0n + ^A_ZX \rightarrow ^{A+1}_ZX^* $$

Each nucleus (apart from Helium-4) gives off a distinct signature of intensities and energies, allowing for the identification of the sample from the γ photon emissions.
2.2 Photon Transport

2.2.1 Photon Reactions

The benchmarking tool analysis relies on three main photon reactions: photoelectric absorption, Compton scattering, and pair production. Although there are other photon reactions, none are an important focus to this work.

**Photoelectric Absorption**

During photoelectric absorption, a photon interacts with a target atom’s electron, departs all of its energy, disappears, and ejects the electron from its bound shell. The photoelectron carries an energy given by equation 2.4 and illustrated by figure 2-1.

\[
E_{\text{e-}} = h\nu - E_b
\]  

(2.4)

Where,

- \(E_b\) is the binding energy of the photoelectron in its original shell
- \(E_{\text{e-}}\) is the energy of the exited photoelectron
- \(h\nu\) is the energy of the incoming photon

![Figure 2-1: Depiction of the Photoelectric Effect](image)

**Compton Scattering**

Compton scattering takes place when a photon interacts with an electron in an atom, it deflected while imparting some of its original energy, and ejects an electron from its orbit. Depending on the scattering angle, the energy transferred to the electron can range from zero to a large fraction of the total photon energy. The energy of the scattered photon and kinetic energy of the scattered electron can be calculated if the energy of the incident photon and incident angle are known by
\[ E'_{\gamma} = \frac{E_{\gamma}}{1 + (1 - \cos \theta)E_{\gamma}/m_e c^2} \]  

(2.5)

Where,

- \( E'_{\gamma} \) is the scattered photon energy
- \( E_{\gamma} \) is the energy of the incident photon
- \( \cos \theta \) is the scattering angle in the lab frame
- \( m_e \) is the mass of the electron
- \( c \) is the speed of light

\[ \text{Pair Production} \]

When an incoming photon exceeds 1.02 MeV, a photon can disappear and create an electron-positron pair. All additional energy carried by the photon above 1.02 MeV is converted into kinetic energy shared by the positron and electron. Although possible at any energy above 1.02 MeV, pair production does not become the dominant reaction until photon energies exceed 5 MeV as shown in Figure 2-5.
Figure 2-4: Depiction of interaction of gamma-rays with a detector medium and their resultant spectra.
2.3 Detector Response

Incident radiation interacting with the detector are modeled in MCNP 6.1 and carry distinct physical signatures (Knoll, 2011). The first order physics alone do not provide a genuine representation of the response from a detector. In order to accurately reproduce a detector response, a detector response function (DRF) must be applied. A detector response function is the expected detector response provided an incoming particle (Gardner and Sood, 2004). During this stage, all non-linear characteristics are removed, allowing the problem to be solved by linear methods.

2.3.1 Spectral Features

Figure 2-6 will serve as an example of the expected features produced by a monoenergetic photon on a detector. The response simulates a 0% resolution detector response from an incoming 6.13 MeV Oxygen-16 decay \( \gamma \)-ray.
A: Full Energy Peak
The full energy peak is equal to the incoming photon energy, 6.13 MeV for this example. The pulse signals that produce this signature occur when the particle enters the detector and deposits all its energy with no escaping secondary particles. This can occur in a singular photoelectric absorption or by a series of reactions. For this reason, the full energy peak can be referred to as the “photoelectric peak”.

B: Compton Edge
Not all events result in full energy deposition. The Compton edge occurs once a photon undergoes a Compton scattering reaction, and then exits the detector without depositing additional energy. The scattering angle determines the energy that is deposited in the detector, ranging from 0° to 180°. From equation 2.6, the maximum energy deposited by a Compton scattering identified as the Compton edge is

$$ \Delta E = E_\gamma - E'_\gamma = 6.13 - \frac{6.13}{1 + (1 - \cos \theta) \cdot \frac{6.13}{0.511}} = 5.88 \text{ MeV} $$  \hspace{1cm} (2.6)
C: Single Escape Peak
In the event a photon creates a pair production reaction, an electron-positron pair is created. The positron will then annihilate inside the detector, creating a 0.511 MeV photon. If the annihilation photon exits the detector without depositing its energy and the full energy of the incoming photon is deposited inside the detector, the result is the single escape peak. The energy of the peak is equal to the full energy peak minus the resting mass energy of an electron, 0.511 MeV.

D: Double Escape Peak
The double escape peak is the result of both annihilation photons escaping the detector. As a result, the detected energy is equal to that of the full energy peak minus the resting mass energy of two electrons, 1.022 MeV.

E: Annihilation Peak
In the event that the incoming particle interacts with a material outside of the detector by a pair production reaction, a resulting annihilation photon can enter the detector and deposit its energy. The annihilation peak appears when the detector is surrounded by a dense material and is equal to 0.511 MeV.

F: Backscattering Peak
The backscattering peak is created when a Compton scattering event occurs outside the detector and the scattered photon reaches the detector and deposits its full energy. The scattering angle occurs over a small range of angles around 180°. This causes the peak to be a range of energies instead of a singular energy peak. The energy for backscattering peak is usually between 200 and 300 KeV. For the case of 180° scatter, the energy of the incoming scattered photon would be

\[
E'_{\gamma} = \frac{6.13}{1 + (1 - \cos \theta) * \frac{6.13}{0.511}} = 0.245 \text{ MeV}
\]  

(2.7)

G: X-Ray Fluorescence Peaks
X-ray fluorescence peaks are not of interest to prompt gamma neutron activation analysis and contributes to a collection of noise signatures that collect below 100 KeV. These peaks are
generated by interactions that occur in the surrounding medium by exciting the target atom. During the de-excitation, characteristic X-ray photons are emitted and enter the detector and deposit their full energy. These peaks complicate the fitting functions, as they can be orders of magnitude higher than other signatures within the spectrum.

**H: X-Ray Escape Peaks**

When the excited atoms discussed above are created within the detector, an X-ray photon can exit the detector. The resulting energy response is equal to the full energy peak minus the energy carried by the exited photon. If the detector material is larger than 1”, these events happen infrequently and do not affect the total response substantially.

**Energy Resolution**

Unfortunately, Figure 2-6 does not accurately represent the true response of even the highest resolution detectors. The energy resolution is dependent on the characteristics of the detector material and electronics. For scintillation detectors, the energy peaks are Gaussian distributed and can be described by the normal distribution

\[ f(E|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} * exp\left(-\frac{(E-\mu)^2}{2\sigma^2}\right) \]  

(2.8)

Where,

- \( E \) is the energy
- \( \mu \) is the peak centroid
- \( \sigma \) is the standard deviation

The common way of determining the standard deviation is by measuring the full width at half maximum (FWHM), or the width of the peak at half of the amplitude. The standard deviation can be calculated by solving for

\[ FWHM \approx 2.355\sigma \]  

(2.9)

It has been demonstrated (Wang and Gardner, 2012) that a subroutine can fit parameters to simplify the FWHM equation to

\[ FWHM = d * E^e \]  

(2.10)

Where,
• $E$ is the energy
• $d, e$ are empirical fitting parameters
CHAPTER 3
Machine Learning
Enhancements

Many modern-day advancements have been made with the assistance of machine learning techniques. Traditional methods of solving linear least squares (LLS) problems can be enhanced by utilizing ready-made packages available on MATLAB and Python coding platforms. All codes used for this investigation have been modified from the sklearn packages in Python.

3.1 Supervised Machine Learning

3.1.1 Linear Least Squares

The linear model and analysis have been thoroughly used and examined over the last half century and remains important. The linear model, given a vector of inputs $X_j$, an output $Y$ can be predicted as

$$\hat{Y} = \beta_0 + \sum_{j=1}^{p} X_j \hat{\beta}_j$$  \hspace{1cm} (3.1)

Where,

- $\beta_0$ is the intercept, also known as the bias in machine learning
- $\hat{Y}$ is the predicted output
\( \hat{\beta}_0 \) can be included in the vector coefficients and a constant variable 1 in X, allowing equation 3.1 to be rewritten as

\[ \hat{Y} = X^T \hat{\beta} + \varepsilon \]  

(3.2)

Where,

- \( X^T \) is the vector or matrix transpose
- \( \hat{Y} \) is the predicted output
- \( \hat{\beta} \) is the linear coefficient
- \( \varepsilon \) is the error

Fitting a linear model to a training data set is popularly done by selecting the \( \beta \) coefficients that minimize the residual sum of squares

\[ RSS(\beta) = \sum_{i=1}^{N} (y_i - x_i^T \beta)^2 \]  

(3.3)

The ordinary least squares estimator can be computed by using the following equation

\[ \hat{\beta}_{OLS} = (X^T X)^{-1} X^T Y \]  

(3.4)

### 3.1.2 Least Absolute Selection and Shrinkage Operator (LASSO)

The least absolute selection and shrinkage operator (LASSO) method became popular as a statistical and modeling method to reduce or eliminate unnecessary variables from a model (Tibshirani, 1996). The LASSO method utilizes tuning parameters to shrink and select variables placed in a linear model by reducing predictive error between in and out of sample tests, also known as test/train splitting in machine learning. LASSO is defined as

\[ \hat{\beta}_{lasso} = \text{argmin}_{\beta \in \mathbb{R}^p} ||y - X\beta||_2^2 + \lambda \sum_{j=1}^{p} |\beta_j| \]  

(3.5)

Or

\[ = \text{argmin}_{\beta \in \mathbb{R}^p} ||y - X\beta||_2^2 + \lambda ||\beta||_1 \]
Where,

- $||y - X\beta||^2$ is the loss function
- $\lambda||\beta||_1$ is a tuning parameter that serves as a penalty
  - Note: when $\lambda = 0$, eq. 3.4 is identical to linear least squares (LLS)

### 3.1.3 Elastic Net

LASSO has been thoroughly investigated since its introduction. While offering many benefits over traditional linear least squares, limitations were found in situations where

- a) In a case where the number of observations ($n$) are less than the number of parameters ($p$) LASSO can select at most $n$ variables
- b) In a case where there are a large number of predictors that are highly correlated, LASSO tends to select only 1, seemingly at random (grouping effect)
- c) In a case where $n>p$ and the predictors are highly correlated; LASSO is dominated by shrinkage methods like Ridge Regression

To remedy these deficiencies, Elastic Net was proposed (Zou and Hastie, 2005). The Elastic Net variable selection method combines the penalty terms used in LASSO and Ridge Regression as

$$\hat{\beta}^\text{ElasticNet} = \arg\min_{\beta \in \mathbb{R}^p} ||y - X\beta||^2 + \lambda_2||\beta||^2 + \lambda_1||\beta||_1$$

(3.6)

Where,

- $||y - X\beta||^2$ is the loss function
- $\lambda_1||\beta||_1$ is a tuning parameter that serves as a penalty from LASSO
- $\lambda_2||\beta||^2$ is a quadratic tuning parameter that serves as a penalty from Ridge Regression
  - Note: when $\lambda_2 = 0$, eq. 3.5 is identical to LASSO
  - Note: when $\lambda_1, \lambda_2 = 0$, eq. 3.5 is identical to linear least squares (LLS)
3.1.4 Coordinate Descent Solutions for LASSO and Elastic Net

Before diving into the detailed derivation for coordinate descent solutions to LASSO and Elastic Net, some background information and notations are necessary (Gauraha, 2018). Consider the standard linear regression equation given as equation 3.2, assume the components of the noise vector are independent and identically distributed. Using subscripts $j$ to denote the jth column of a dataset. Assuming that the design matrix $X$ is fixed, the data is adjusted to be centered, and the predictors are standardized such that

\[
\sum_{i=1}^{n} Y_i = 0, \sum_{i=1}^{n} (X_j)_i = 0 \text{ and } \frac{1}{n} X_j^T X_j = 1 \text{ for all } j = 1, \ldots, p.
\]  

(3.7)

The $l_{0,1,2}$-norms are defined as

\[
||\beta||_0 = \sum_{j=1}^{p} I(\beta_j \neq 0)
\]

\[
||\beta||_1 = \sum_{j=1}^{p} |\beta_j|
\]

\[
||\beta||_2^2 = \sum_{j=1}^{p} \beta_j^2
\]

(3.8)

Then, the soft-thresholding operator can be defined as follows

\[
S_\lambda(x) = \begin{cases} 
  x + \lambda & \text{if } x < -\lambda \\
  0 & \text{if } |x| \leq \lambda \\
  x - \lambda & \text{if } x > \lambda
\end{cases}
\]

(3.9)
3.1.4.1 LASSO Single Variable Case

Before moving to a case involving multiple variables, a single variable case is considered. For this case, $p=1$ and $Y = X_1 \beta_1 + \varepsilon$, and the optimization problem can be written as

$$
arg\min_{\beta \in \mathbb{R}^p} \frac{1}{n} ||Y - X_1 \beta_1||_2^2 + \lambda |\beta_1|
$$

(3.10)

Assuming $\hat{\beta}_1$ is a solution to equation 3.10, then the sub-differential must contain zero, meaning

$$
-\frac{2}{n} X_1^T (Y - X_1 \hat{\beta}_1) + \lambda \ast sign(\hat{\beta}_1) = 0,
$$

(3.11)

Which can be rewritten as

$$
\frac{1}{n} X_1^T (Y - X_1 \hat{\beta}_1) = \frac{\lambda}{2} sign(\hat{\beta}_1)
$$
Note that since we are assuming the predictors are standardized, \( \frac{1}{n} X_1^T X_1 = 1 \),

\[
\hat{\beta}_1 = \frac{1}{n} X_1^T Y - \frac{\lambda}{2} \text{sign}(\hat{\beta}_1) \quad (3.12)
\]

\[
\hat{\beta}_1 = \begin{cases} 
\frac{1}{n} X_1^T Y + \frac{\lambda}{2} & \text{if } \frac{1}{n} X_1^T Y < -\frac{\lambda}{2} \\
0 & \text{if } \frac{1}{n} X_1^T Y \leq \frac{\lambda}{2} \\
\frac{1}{n} X_1^T Y - \frac{\lambda}{2} & \text{if } \frac{1}{n} X_1^T Y > \frac{\lambda}{2}
\end{cases}
\]

An alternative interpretation is that \( \hat{\beta}_1 = \frac{1}{n} X_1^T Y \) is soft-thresholded by \( \frac{\lambda}{2} \) such that

\[
\hat{\beta}_1 = \frac{1}{\tau} \left( \frac{1}{n} X_1^T Y \right) \quad (3.13)
\]

Therefore, the LASSO estimator for a single variable case can be computed by soft-thresholding the OLS estimator by \( \frac{\lambda}{2} \) or

\[
\hat{\beta}_1 = \frac{1}{\tau} \left( \hat{B}_{OLS} \right) \quad (3.14)
\]

Where \( \hat{B}_{OLS} = \frac{1}{n} X_1^T Y \).

### 3.1.4.2 Coordinate Descent for LASSO

In order to treat LASSO algorithmically, the objective function must be split into a differentiable part \( f_d = ||Y - X_j \beta_j||_2^2 \) and a non-differentiable part \( f_c = \sum_{j=1}^{P} |\beta_j| \). The non-differentiable component \( f_c = \sum_{j=1}^{P} |\beta_j| \) is convex in each coordinate, allowing for a coordinate wise minimization to be utilized (Gauraha, 2018). Section 3.1.4.1 demonstrated that with a single predictor, the LASSO solution has a closed for solution with a soft-threshold version of the ordinary least squares estimate. Building on this, a coordinate descent algorithm for the LASSO can be implemented as follows.

Coordinate descent is an iterative method that solves one variable iteratively, while holding all other variables constant. For each coordinate sub-problem, each component of \( \beta \) is fixed except for the jth component \( \beta_j \). By denoting \( X_j \) as the jth column of \( X \) and \( X_{-j} \) denote all of the columns except for the jth column, then the problem can be rewritten as
Next, we define $r_j := Y - X_j \beta_{-j}$ as the partial residual or the difference between the actual response $Y$ and the fitted model that excludes variable $X_j$. The solution above becomes the univariate LASSO problem with vector $r_j$ as the response variable

$$
\text{argmin}_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{n} \| r_j - X_j \beta_j \|_2^2 + \lambda |\beta_j| + \lambda \sum_{l \neq j} |\beta_l| \right\}
$$

(3.16)

Now suppose $\hat{\beta}_j$ is a solution to the optimization problem above. Then the stationary condition yields the following

$$
-\frac{2}{n} X_j^T (r_j - X_j \hat{\beta}_j) + \lambda \cdot \text{sign}(\hat{\beta}_j) = 0,
$$

(3.17)

$$
\frac{1}{n} r_j^T X_j - \hat{\beta}_j = \frac{\lambda}{2} \text{sign}(\hat{\beta}_j)
$$

The OLS estimator for the $j$th variable can then be computed as $\hat{\beta}_{OLS,j} = \frac{1}{n} r_j^T X_j$. The univariate LASSO solution can then be computed by soft-thresholding the OLS estimator as

$$
\hat{\beta}_j = S_{\frac{\lambda}{2}}(\hat{\beta}_{OLS,j})
$$

(3.18)

Table 3.1 demonstrates the full coordinate descent algorithm for LASSO. The dataset is loaded and initialized such that $\beta = 0$. Then for each $j$ term, the single variable LASSO solution is computed. The entire process is repeated until $\hat{\beta} = \beta$. 
Table 3-1: Full LASSO Coordinate Descent Algorithm

**LASSO Coordinate Descent Algorithm**

**Input:** dataset \((Y, X)\)

**Output:** \(\hat{\beta} = \text{LASSO estimated vector of regression coefficients}\)

Initialize \(\beta = 0\)

repeat

   for each \(j \in \{1, \ldots, p\}\) do

      Compute the partial residual \(r_j\), where

      \[
      r_j = Y - \sum_{i \neq j} X_i \beta_i
      \]

      Compute the OLS coefficient for single predictor

      \[
      (\hat{B}_{OLS})_j = \frac{1}{n} r_1^T X_j
      \]

      Update \(\beta_j\) (LASSO solution: single variable case)

      \[
      \beta_j = S_{\frac{\lambda}{2}}((\hat{B}_{OLS})_j)
      \]

   end

until convergence;

\(\hat{\beta} = \beta\)

Return \(\hat{\beta}\)

3.1.4.3 Coordinate Descent for Elastic Net

The derivation and steps to calculate the Elastic Net penalty via coordinate descent are similar to those taken to calculate the LASSO penalty (Yang, 2013). The second order penalty adds an additional term to the LASSO solution such that

\[
\arg\min_{\beta \in \mathbb{R}^p} \frac{1}{n} ||Y - X_1 \beta_1||_2^2 + P_{\lambda,a}(\beta)
\]  

(3.19)
Where $P_{\lambda,\alpha}(\beta)$ is the Elastic Net penalty defined as

$$P_{\lambda,\alpha}(\beta) = \lambda \sum_{j=1}^{p} p_{\alpha}(\beta_j) = \lambda \sum_{j=1}^{p} \left[ \frac{1}{2} (1 - \alpha)\beta_j^2 + \alpha |\beta_j| \right]$$

Note that when $\alpha = 1$, the Elastic Net reduces to the LASSO equation. When each predictor shows a strong correlation, some $\alpha < 1$ should be used. For each fixed $\lambda$, coordinate descent is used to solve the Elastic Net. Once again, we define a current residual $r_j := Y - X_{-j} \beta_{-j}$ that excludes the jth term from each calculation. To update the estimate for $\beta_j$, the univariate Elastic Net problem is solved by

$$\hat{\beta}_j = \arg\min_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{n} |r_j - X_j \beta_j|_2^2 + \lambda p_{\alpha}(\beta_j) \right\}$$  \hspace{1cm} (3.20)

The soft threshold is applied, leading to

$$\hat{\beta}_j = S\left( \frac{1}{n} r_j X_j + \beta_j, \lambda \alpha \right) \hspace{1cm} (3.21)$$

Table 3.2 demonstrates the full coordinate descent algorithm for Elastic Net. The dataset is loaded and initialized such that $\beta = 0$. Then for each j term, the single variable Elastic Net solution is computed. The entire process is repeated until $\hat{\beta} = \beta$.
**Table 3.2: Full Elastic Net Coordinate Descent Algorithm**

**Input:** dataset (\(Y, X\))

**Output:** \(\hat{\beta} := \) Elastic Net estimated vector of regression coefficients

Initialize \(\beta = 0\)

repeat

  for each \(j \in \{1, ..., p\}\) do

    Compute the partial residual \(r_j\), where

    \[
    r_j = Y - \sum_{i \neq j} X_i \beta_i
    \]

    Update \(\beta_j\) (Elastic Net solution: single variable case)

    \[
    \hat{\beta}_j = \frac{S\left(\frac{1}{n} r^T X_j + \beta_j, \lambda \alpha\right)}{1 + \lambda (1 - \alpha)}
    \]

  end

until convergence;

\(\hat{\beta}_j = \beta_j\)

Return \(\hat{\beta}\)

---

### 3.1.5 Cross Validation

Cross validation is a method to perform out-of-sample testing to assess the results of statistical analysis on an independent data set. After the experimental and simulated data are processed and separated into \(X\) and \(Y\) vectors, the full data set is split into testing and training subsets via the holdout method shown in figure 3-2. As a result of splitting the data, additional bias is introduced to each solution, as different parts of the data are either included or removed from the model selection process. Cross validation is used to perform the test-train split process multiple times, averaging each solution to provide a less biased solution as seen in figure 3-3. Cross validation is used to find the optimal normalization parameter for both LASSO and Elastic Net.
Figure 3-2: Holdout method for test-train split

Figure 3-3: Cross validation holdout
CHAPTER 4

Kansas State Experiment

4.1 Data Collection

4.1.1 Kansas State Experimental Data

In section 1.2, the Kansas State University benchmarking tool and experimental facility were described. Five separate experimental runs were conducted for tap water, pure sand, sand with water, pure limestone, and limestone with water. For each of these experimental runs, the data collection sequence involved:

1) Source calibration runs to adjust gain on detection systems
2) Pre-run background tests (5 minutes)
3) Live D-T run (1 hour)
4) Post-run background tests (5 minutes)

The data collected during each of these runs was processed by Kansas State University and converted into counts per channel text files for each detector. Additional binary files were provided that have time dependent information for the pulsing sequence and detector responses with respect to time.

The counts per channel data files must be processed and converted to energy to match the simulated responses. A second order polynomial is used for fitting purposes by

\[ \text{Energy} = a + b \times \text{channel} + c \times \text{channel}^2 \]  

(4.1)
4.1.2 Simulated Data

In order to simulate an accurate detector response, extensive (~10⁹ particles) MCNP 6.1 calculations were conducted with accurate details of the detector, tool, test chamber, and surrounding medium geometry and materials. Libraries were created by using F8 tallies for each detector and medium (water, sand, limestone, etc.). To accurately model the detector response, Gaussian broadening functions were used in order to take the pulse response and broaden the data to match the FWHM found using the calibration sources.

![Gaussian Broadening](image)

Figure 4-1: F8 tally simulated response and Gaussian broadened detector response

4.1.3 Simulated Example

Prior to running a full example with data from Kansas State University, a simulated example was conducted to demonstrate the capabilities of each code. Using simulated data, a salt water test case was created by combining a combination of water, sodium, and chlorine libraries. Random Poisson distributed noise was then applied to the test case to simulate the random effects found in true examples. Five total libraries were used as training data sets (water, sodium, chlorine, iron, and copper) to train the model versus the test data set containing salt water. Using 10-fold
cross validation, the model was correctly trained to fit only the 3 libraries that contribute to the full spectrum, while providing a zero contribution for the iron and copper libraries. Figures 4-2 thru 4-7 demonstrate how the tuning parameters select the best model and the final fits for LASSO and Elastic Net.

**Figure 4-2:** Cross validation normalization parameter selection for LASSO

**Figure 4-3:** LASSO model selection coefficients by changing normalization parameter
**Figure 4-4:** LASSO salt water simulation fit

**Figure 4-5:** Cross validation normalization parameter selection for Elastic Net
Figure 4-6: Elastic Net model selection by changing normalization parameter

Figure 4-7: Elastic Net salt water simulation fit
When the normalization parameter is increased, the penalty for each term becomes greater, allowing the shrinkage and removal of parameters. The MSE at each alpha parameter is compared, settling on the best overall fit for the final solution. Without putting the output of the LASSO and Elastic Net fits into an OLS program for a final fit, table 4-1 displays the relative error of each method averaged over 10 runs.

<table>
<thead>
<tr>
<th></th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Elastic Net</td>
</tr>
<tr>
<td>Water</td>
<td>5.01%</td>
</tr>
<tr>
<td>Na</td>
<td>2.95%</td>
</tr>
<tr>
<td>Cl</td>
<td>7.95%</td>
</tr>
</tbody>
</table>

### 4.2 Methods and Improvements

#### 4.2.1 Full Procedure

Before any data analysis can take place, a variety of preprocessing and post processing of data is necessary (Fig. 4-8). Experimental and simulated data are generated at Kansas State and North Carolina State, respectively. The experimental data is processed and separated into counts per channel text files for each detector type, as well as binary files with time dependent data. The detector data is converted into energy bins using calibration sources for empirical FWHM calculations.

The simulated data is generated using MCNP 6.1 using the F8 tally. The nonlinear response in the Gaussian broadening detector response function is addressed, resulting in a final library spectrum.
Each library is added to a single file and used to train the fitting model. A 10-fold cross validation process helps reduce the overall bias in model selection. For the test/train split, 90% of the data is used each time for training, while 10% of the data is held out to test the model. LASSO and Elastic Net are applied to select the best model that reduces a loss function (MSE). Once the final solution is reached, the output from LASSO and Elastic Net are used as initial guesses in an ordinary least squares fitting using CEARLLS.

4.2.2 Early Lessons Learned

A pure water trial was conducted and processed by the procedure laid out in section 4.2.1. Upon completing the final fitting, several deviations were observed as seen in Figure 4-9. In the high energy range, above 7 MeV, differences between the simulated and experimental response are expected, as the error in each channel is high from the low count rate. The hydrogen peak and oxygen peaks fit well to the simulations, however, the region below 2 MeV does not have a proper fitting. The proposed solution was to look at the activation of the NaI crystal (Gardner, 2000).
To test this theory, a library response for activated Sodium and Iodine are added to the fitting libraries (Fig. 4-10). Although this did improve the overall fit, it did not completely resolve the discrepancies.
To completely understand the nature of the activated (delayed) response, the time dependent D-T data is necessary. The primary advantage of using a PNG is the ability to read signatures that are prompt and delayed by the response times. The PNG is triggered using a firing sequence from the generator and a pulse of neutrons is emitted. After the pulse, there is a window of time before the next initialization where the neutrons have died off, and the only remaining signatures are from delayed activation (Figs. 4-11, 4-12).

![Figure 4-11: Firing sequence and measured response](image_url)
4.3 Kansas State Experimental Results

Five separate trials were conducted to provide an experimental basis for this investigation. A water, sand, sand with water, limestone, and limestone with water trial were conducted to provide a broad range of materials and conditions to simulate, fit, and compare to methods currently implemented in the oil well logging industry. Using the post run background measurements, the delayed response is extracted and removed from the final response. The gaussian broadening parameters used for each of these trials was extracted by the method described in section 2.3 as

\[ FWHM = 0.031 \times E^{0.5} \] (4.2)

MCNP simulated responses are separated into water, sand, limestone, iron, and copper libraries for near and far detectors and broadened by the parameters in eq. 4.2. The variable selection codes take the experimental response for each detector separately and provide a model prediction against the five input libraries for that detector. This process is repeated for both the near and far detectors for each trial run, followed by a final ordinary least squares fitting and error analysis. The first 200 and final 548 channels are ignored from the variable selection and final fitting steps.
4.3.1 Water Trial

The first trial was conducted using tap water. The channel to energy conversion was accomplished by identifying the peak centroids in the sample and adjusting by

\[
E_{nergy}(MeV) = -0.01 + 0.005 \times \text{channel} + 2 \times 10^{-7} \times \text{channel}^2
\] (4.3)

The cross-validation curve (figs. 4-13, 4-17, 4-21, 4-25) demonstrates the process by which the normalization parameter is selected by LASSO and Elastic Net for the near and far detectors. The optimum normalization parameter is presented on the regularization path (figs. 4-14, 4-18, 4-22, 4-26) tracking the coefficients for each library as the normalization parameter changes. The output from the LASSO and Elastic Net codes are presented in figures 4-15, 4-19, 4-23, and 4-27 using only channels 200 thru 1500. The remaining figures provide the full fit using the coefficients determined using the truncated dataset.

![Mean square error on each fold: coordinate descent](image)

*Figure 4-13:* Cross validation normalization parameter selection for the LASSO near detector water trial
Figure 4-14: LASSO model selection coefficients by changing the normalization parameter for the near detector water trial

Figure 4-15: LASSO fit for the near detector water trial
Figure 4-16: LASSO full fit for the near detector water trial

Figure 4-17: Cross validation normalization parameter selection for the Elastic Net near detector water trial
Figure 4-18: Elastic Net model selection coefficients by changing the normalization parameter for the near detector water trial

Figure 4-19: Elastic Net fit for the near detector water trial
Figure 4-20: Elastic Net full fit for the near detector water trial

Figure 4-21: Cross validation normalization parameter selection for the LASSO far detector water trial
Figure 4-22: LASSO model selection coefficients by changing the normalization parameter for the far detector water trial

Figure 4-23: LASSO fit for the far detector water trial
Figure 4-24: LASSO full fit for the far detector water trial

Figure 4-25: Cross validation normalization parameter selection for the Elastic Net far detector water trial
**Figure 4-26:** Elastic Net model selection coefficients by changing the normalization parameter for the far detector water trial

**Figure 4-27:** Elastic Net fit for the far detector water trial
The results show that both LASSO and Elastic Net perform similarly for the near and far detectors. Each correctly identifies the presence of water alone for the near detector, while both misidentifying a copper contribution for the far detectors. Table 4-2 lists the optimal normalization parameters for each case identified by cross validation. The results for the variable selection process are used as inputs for the final ordinary least squares fitting using the cearlls code. Figures 4-29 and 4-30 display the final fitting and residuals for the near and far detector, respectively. Figure 4-31 shows the near and far final fits together. Tables 4-3, 4-4 provide the chi-squared value, fitting coefficients, and corresponding error for the near and far detectors.

<table>
<thead>
<tr>
<th>Water Normalization Parameters</th>
<th>Near Detector</th>
<th>Far Detector</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LASSO</strong></td>
<td>0.464</td>
<td>0.136</td>
</tr>
<tr>
<td><strong>Elastic Net</strong></td>
<td>2.783</td>
<td>0.024</td>
</tr>
</tbody>
</table>
Figure 4-29: Linear least squares fit and residual for the near detector water trial

Figure 4-30: Linear least squares fit and residual for the far detector water trial
Figure 4-31: Linear least squares fit for near and far detector water trials

Table 4-3: Linear coefficients and error for water near detector

<table>
<thead>
<tr>
<th>Water Linear Least Squares Results – Near Detector</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Chi-Squared = 99.3</strong></td>
</tr>
<tr>
<td>Water</td>
</tr>
<tr>
<td>Sand</td>
</tr>
<tr>
<td>Limestone</td>
</tr>
<tr>
<td>Iron</td>
</tr>
<tr>
<td>Copper</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>-----------------</td>
</tr>
<tr>
<td>Water</td>
</tr>
<tr>
<td>Sand</td>
</tr>
<tr>
<td>Limestone</td>
</tr>
<tr>
<td>Iron</td>
</tr>
<tr>
<td>Copper</td>
</tr>
</tbody>
</table>

### 4.3.2 Sand Trial

The next trial conducted involved pure sand. No chemical or other analysis was performed on the material, so it is assumed that the makeup is SiO$_2$. The channel to energy conversion was accomplished by identifying the peak centroids in the sample and adjusting by

$$\text{Energy} (\text{MeV}) = -0.051 + 0.00511 \times \text{channel} + 1 \times 10^{-7} \times \text{channel}^2$$  (4.4)

All other parameters and order of figures are consistent with those from section 4.3.1. As a test to the versatility of LASSO and Elastic Net, each spectrum was shifted by 5 channels in the sand trial to demonstrate how each solves an ill conditioned case.
**Figure 4-32:** Cross validation normalization parameter selection for the LASSO near detector sand trial

**Figure 4-33:** LASSO model selection coefficients by changing the normalization parameter for the near detector sand trial
Figure 4-34: LASSO fit for the near detector sand trial

Figure 4-35: LASSO full fit for the near detector sand trial
Figure 4-36: Cross validation normalization parameter selection for the Elastic Net near detector sand trial

Figure 4-37: Elastic Net model selection coefficients by changing the normalization parameter for the near detector sand trial
Figure 4-38: Elastic Net fit for the near detector sand trial

Figure 4-39: Elastic Net full fit for the near detector sand trial
Figure 4-40: Cross validation normalization parameter selection for the LASSO far detector sand trial

Figure 4-41: LASSO model selection coefficients by changing the normalization parameter for the far detector sand trial
Figure 4-42: LASSO fit for the far detector sand trial

Figure 4-43: LASSO full fit for the far detector sand trial
Figure 4-44: Cross validation normalization parameter selection for the Elastic Net far detector sand trial

Figure 4-45: Elastic Net model selection coefficients by changing the normalization parameter for the far detector sand trial
Figure 4-46: Elastic Net fit for the far detector sand trial

Figure 4-47: Elastic Net full fit for the far detector sand trial
The results show that both LASSO and Elastic Net recognize the presence of both sand and water in the near detector, while also detecting iron in the far detector. The detection of water was attributed by the Kansas State University researchers as high humidity from running the test in the summer months, as well as not fully evacuating the test chamber of water before the next test. Table 4-5 lists the optimal normalization parameters for each case identified by cross validation. The results for the variable selection process are used as inputs for the final ordinary least squares fitting using the cearlls code. Figures 4-48 and 4-49 display the final fitting and residuals for the near and far detector, respectively. Figure 4-50 shows the near and far final fits together. Tables 4-6, 4-7 provide the chi-squared value, fitting coefficients, and corresponding error.

**Table 4-5:** Optimal normalization parameters for sand trial

<table>
<thead>
<tr>
<th>Sand Normalization Parameters</th>
<th>Near Detector</th>
<th>Far Detector</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LASSO</strong></td>
<td>0.396</td>
<td>1.050</td>
</tr>
<tr>
<td><strong>Elastic Net</strong></td>
<td>0.526</td>
<td>0.060</td>
</tr>
</tbody>
</table>

**Figure 4-48:** Linear least squares fit and residual for the near detector sand trial
Figure 4-49: Linear least squares fit and residual for the far detector sand trial

Figure 4-50: Linear least squares fit for near and far detector sand trials
Table 4-6: Linear coefficients and error for sand near detector

<table>
<thead>
<tr>
<th></th>
<th>Water Linear Least Squares Results – Near Detector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chi-Squared</td>
<td>88.4</td>
</tr>
<tr>
<td></td>
<td><strong>Coefficients</strong></td>
</tr>
<tr>
<td>Water</td>
<td>79.94</td>
</tr>
<tr>
<td>Sand</td>
<td>437.37</td>
</tr>
<tr>
<td>Limestone</td>
<td>NA</td>
</tr>
<tr>
<td>Iron</td>
<td>NA</td>
</tr>
<tr>
<td>Copper</td>
<td>NA</td>
</tr>
</tbody>
</table>

Table 4-7: Linear coefficients and error for sand far detector

<table>
<thead>
<tr>
<th></th>
<th>Water Linear Least Squares Results – Far Detector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chi-Squared</td>
<td>27.6</td>
</tr>
<tr>
<td></td>
<td><strong>Coefficients</strong></td>
</tr>
<tr>
<td>Water</td>
<td>203.90</td>
</tr>
<tr>
<td>Sand</td>
<td>210.55</td>
</tr>
<tr>
<td>Limestone</td>
<td>NA</td>
</tr>
<tr>
<td>Iron</td>
<td>NA</td>
</tr>
<tr>
<td>Copper</td>
<td>NA</td>
</tr>
</tbody>
</table>

4.3.3 Sand with Water Trial

The next trial conducted involved sand with added water. No chemical or other analysis was performed on the material, so it is assumed that the makeup is SiO₂. The channel to energy conversion was accomplished by identifying the peak centroids in the sample and adjusting by

\[
Energy(MeV) = -0.051 + 0.00511 \times channel + 1e^{-7} \times channel^2
\]  (4.5)

All other parameters and order of figures are consistent with those from section 4.3.1.
**Figure 4-51:** Cross validation normalization parameter selection for the LASSO near detector sand and water trial

**Figure 4-52:** LASSO model selection coefficients by changing the normalization parameter for the near detector sand and water trial
**Figure 4-53:** LASSO fit for the near detector sand and water trial

**Figure 4-54:** LASSO full fit for the near detector sand and water trial
Figure 4-55: Cross validation normalization parameter selection for the Elastic Net near detector sand and water trial

Figure 4-56: Elastic Net model selection coefficients by changing the normalization parameter for the near detector sand and trial
Figure 4-57: Elastic Net fit for the near detector sand and water trial

Figure 4-58: Elastic Net full fit for the near detector sand and water trial
Figure 4-59: Cross validation normalization parameter selection for the LASSO far detector sand and water trial

Figure 4-60: LASSO model selection coefficients by changing the normalization parameter for the far detector sand and water trial
Figure 4-61: LASSO fit for the far detector sand and water trial

Figure 4-62: LASSO full fit for the far detector sand and water trial
Figure 4-63: Cross validation normalization parameter selection for the Elastic Net far detector sand and water trial

Figure 4-64: Elastic Net model selection coefficients by changing the normalization parameter for the far detector sand and water trial
Figure 4-65: Elastic Net fit for the far detector sand and water trial

Figure 4-66: Elastic Net full fit for the far detector sand and water trial
The results show that both LASSO and Elastic Net recognize the presence of both sand and water in the near and far detectors. 3 of the 4 tests also include small amounts of iron or copper. Table 4-8 lists the optimal normalization parameters for each case identified by cross validation. The results for the variable selection process are used as inputs for the final ordinary least squares fitting using the cearlls code. Figures 4-67 and 4-68 display the final fitting and residuals for the near and far detector, respectively. Figure 4-69 shows the near and far final fits together. Tables 4-9, 4-10 provide the chi-squared value, fitting coefficients, and corresponding error.

<table>
<thead>
<tr>
<th>Table 4-8: Optimal normalization parameters for sand and water trial</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Sand and Water Normalization Parameters</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Near Detector</strong></td>
</tr>
<tr>
<td>LASSO</td>
</tr>
<tr>
<td>Elastic Net</td>
</tr>
</tbody>
</table>

**Figure 4-67:** Linear least squares fit and residual for the near detector sand and water trial
Figure 4-68: Linear least squares fit and residual for the far detector sand and water trial

Figure 4-69: Linear least squares fit for near and far detector sand and water trials
Table 4-9: Linear coefficients and error for sand and water near detector

<table>
<thead>
<tr>
<th></th>
<th>Coefficients</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Water</strong></td>
<td>164.20</td>
<td>0.48</td>
</tr>
<tr>
<td><strong>Sand</strong></td>
<td>247.83</td>
<td>0.20</td>
</tr>
<tr>
<td><strong>Limestone</strong></td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td><strong>Iron</strong></td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td><strong>Copper</strong></td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>

Table 4-10: Linear coefficients and error for sand and water far detector

<table>
<thead>
<tr>
<th></th>
<th>Coefficients</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Water</strong></td>
<td>125.89</td>
<td>1.34</td>
</tr>
<tr>
<td><strong>Sand</strong></td>
<td>152.51</td>
<td>0.62</td>
</tr>
<tr>
<td><strong>Limestone</strong></td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td><strong>Iron</strong></td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td><strong>Copper</strong></td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>

4.3.4 Limestone Trial

The next trial conducted involved pure limestone. No chemical or other analysis was performed on the material, so it is assumed that the makeup is CaCO₃, SiO₂, and SiO₄. The channel to energy conversion was accomplished by identifying the peak centroids in the sample and adjusting by

\[
Energy(MeV) = -0.012 + 0.00492 \times channel + 2e^{-7} \times channel^2
\]  (4.6)

All other parameters and order of figures are consistent with those from section 4.3.1.
Figure 4-70: Cross validation normalization parameter selection for the LASSO near detector limestone trial

Figure 4-71: LASSO model selection coefficients by changing the normalization parameter for the near detector limestone trial
Figure 4-72: LASSO fit for the near detector limestone trial

Figure 4-73: LASSO full fit for the near detector limestone trial
Figure 4-74: Cross validation normalization parameter selection for the Elastic Net near detector limestone trial

Figure 4-75: Elastic Net model selection coefficients by changing the normalization parameter for the near detector limestone trial
**Figure 4-76:** Elastic Net fit for the near detector limestone trial

**Figure 4-77:** Elastic Net full fit for the near detector limestone trial
Figure 4-78: Cross validation normalization parameter selection for the LASSO far detector limestone trial

Figure 4-79: LASSO model selection coefficients by changing the normalization parameter for the far detector limestone trial
Figure 4-80: LASSO fit for the far detector limestone trial

Figure 4-81: LASSO full fit for the far detector limestone trial
**Figure 4-82:** Cross validation normalization parameter selection for the Elastic Net far detector limestone trial

**Figure 4-83:** Elastic Net model selection coefficients by changing the normalization parameter for the far detector limestone trial
Figure 4-84: Elastic Net fit for the far detector limestone trial

Figure 4-85: Elastic Net full fit for the far detector limestone trial
The results show that both LASSO and Elastic Net recognize the presence of limestone, sand, and water in the near and far detectors. The inclusion of water in each of the results has been attributed to a light rain sustained during the loading of the material. 3 of the 4 tests also include small amounts of iron or copper. Table 4-11 lists the optimal normalization parameters for each case identified by cross validation. The results for the variable selection process are used as inputs for the final ordinary least squares fitting using the cearlls code. Figures 4-86 and 4-87 display the final fitting and residuals for the near and far detector, respectively. Figure 4-88 shows the near and far final fits together. Tables 4-12 and 4-13 provide the chi-squared value, fitting coefficients, and corresponding error.

Table 4-11: Optimal normalization parameters for limestone trial

<table>
<thead>
<tr>
<th></th>
<th>Near Detector</th>
<th>Far Detector</th>
</tr>
</thead>
<tbody>
<tr>
<td>LASSO</td>
<td>5.384</td>
<td>1.163</td>
</tr>
<tr>
<td>Elastic Net</td>
<td>0.419</td>
<td>0.118</td>
</tr>
</tbody>
</table>

Figure 4-86: Linear least squares fit and residual for the near detector limestone trial
Figure 4-87: Linear least squares fit and residual for the far detector limestone trial

Figure 4-88: Linear least squares fit for near and far detector limestone trials
### Table 4-12: Linear coefficients and error for limestone near detector

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Water</strong></td>
<td>104.44</td>
</tr>
<tr>
<td><strong>Sand</strong></td>
<td>139.82</td>
</tr>
<tr>
<td><strong>Limestone</strong></td>
<td>230.1</td>
</tr>
<tr>
<td><strong>Iron</strong></td>
<td>NA</td>
</tr>
<tr>
<td><strong>Copper</strong></td>
<td>NA</td>
</tr>
</tbody>
</table>

Chi-Squared = 26.7

### Table 4-13: Linear coefficients and error for limestone far detector

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Water</strong></td>
<td>75.14</td>
</tr>
<tr>
<td><strong>Sand</strong></td>
<td>90.42</td>
</tr>
<tr>
<td><strong>Limestone</strong></td>
<td>171.14</td>
</tr>
<tr>
<td><strong>Iron</strong></td>
<td>NA</td>
</tr>
<tr>
<td><strong>Copper</strong></td>
<td>NA</td>
</tr>
</tbody>
</table>

Chi-Squared = 18.2

### 4.3.5 Limestone with Water Trial

The final trial conducted involved limestone with added water. No chemical or other analysis was performed on the material, so it is assumed that the makeup is CaCO3, SiO2, and water. The channel to energy conversion was accomplished by identifying the peak centroids in the sample and adjusting by

\[
E_{nergy}(MeV) = -0.046 + 0.005063 \times channel + 2e^{-7} \times channel^2
\]  

All other parameters and order of figures are consistent with those from section 4.3.1.
Figure 4-89: Cross validation normalization parameter selection for the LASSO near detector limestone and water trial

Figure 4-90: LASSO model selection coefficients by changing the normalization parameter for the near detector limestone and water trial
Figure 4-91: LASSO fit for the near detector limestone and water trial

Figure 4-92: LASSO full fit for the near detector limestone and water trial
Figure 4-93: Cross validation normalization parameter selection for the Elastic Net near detector limestone and water trial

Figure 4-94: Elastic Net model selection coefficients by changing the normalization parameter for the near detector limestone and water trial
Figure 4-95: Elastic Net fit for the near detector limestone and water trial

Figure 4-96: Elastic Net full fit for the near detector limestone and water trial
Figure 4-97: Cross validation normalization parameter selection for the LASSO far detector limestone and water trial

Figure 4-98: LASSO model selection coefficients by changing the normalization parameter for the far detector limestone and water
Figure 4-99: LASSO fit for the far detector limestone and water trial

Figure 4-100: LASSO full fit for the far detector limestone and water trial
Figure 4-101: Cross validation normalization parameter selection for the Elastic Net far detector limestone and water trial

Figure 4-102: Elastic Net model selection coefficients by changing the normalization parameter for the far detector limestone and water trial
Figure 4-103: Elastic Net fit for the far detector limestone and water trial

Figure 4-104: Elastic Net full fit for the far detector limestone and water trial
The results show that both LASSO and Elastic Net recognize the presence of limestone, sand, and water in the near and far detectors in 3 of the 4 detectors. Each of the tests also include large amounts of copper. Table 4-14 lists the optimal normalization parameters for each case identified by cross validation. The results for the variable selection process are used as inputs for the final ordinary least squares fitting using the cearlls code. Figures 4-105 and 4-106 display the final fitting and residuals for the near and far detector, respectively. Figure 4-107 shows the near and far final fits together. Tables 4-15 and 4-16 provide the chi-squared value, fitting coefficients, and corresponding error.

<table>
<thead>
<tr>
<th>Table 4-14: Optimal normalization parameters for limestone and water trial</th>
</tr>
</thead>
<tbody>
<tr>
<td>Limestone with Water Normalization Parameters</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Near Detector</td>
</tr>
<tr>
<td>Elastic Net</td>
</tr>
</tbody>
</table>

Figure 4-105: Linear least squares fit and residual for the near detector limestone and water trial
Figure 4-106: Linear least squares fit and residual for the far detector limestone and water trial

Figure 4-107: Linear least squares fit for near and far detector limestone and water trial
### Table 4-15: Linear coefficients and error for limestone and water near detector

<table>
<thead>
<tr>
<th></th>
<th>Coefficients</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>140.80</td>
<td>0.51</td>
</tr>
<tr>
<td>Sand</td>
<td>90.48</td>
<td>1.77</td>
</tr>
<tr>
<td>Limestone</td>
<td>114.66</td>
<td>1.76</td>
</tr>
<tr>
<td>Iron</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>Copper</td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>

Chi-Squared = 34.2

### Table 4-16: Linear coefficients and error for limestone and water far detector

<table>
<thead>
<tr>
<th></th>
<th>Coefficients</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>96.77</td>
<td>1.91</td>
</tr>
<tr>
<td>Sand</td>
<td>64.89</td>
<td>3.64</td>
</tr>
<tr>
<td>Limestone</td>
<td>71.21</td>
<td>4.61</td>
</tr>
<tr>
<td>Iron</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>Copper</td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>

Chi-Squared = 10.2

### 4.4 Discussion

The LASSO and Elastic Net variable selection techniques perform well for both the sand and water trials. The results with the limestone trials show some of the problems if the libraries or data collection are off by any significant amount. During a conversation with oil industry experts, it was noted that calcium cross sections have errors, possibly contributing to the difficulties in the variable selection process for limestone. Additionally, they stated that they are no longer using the far detectors to determine the density of the materials. Further tests should remove the far gamma detector. Improvements continue to be made by both the NC State group and the Kansas State group. Aaron Feinberg is working on a Bayesian approach to fit the non-linear components instead of the basic calculations currently being used. Long Vo is working on separating the time dependent data to improve the background contribution.
CHAPTER 5
Radioisotope Identification
Device Algorithm

5.1 Data Collection

Six radioisotope sources (Ba-133, Na-22, Cs-137, Co-57, Co-60, and Mn-54) were simulated at a distance of 10 cm from the detector face using geometry from a standard 3x3 NaI detector, each with an energy below 1.5 MeV (figs. 5-1, 5-2). Some of the most difficult problems in radioisotope identification involve shielding, masking, and convolution. The masking problem is when several higher energy radioisotopes reduce the signature of a lower energy source, drowning out the contribution in the Compton continuum. Convolved peaks are a major concern in techniques involving peak identification. LASSO and Elastic Net provide a full spectrum analysis, offering a potential solution to this problem. Finally, shielding introduces distortions to the gamma response depending on the materials used, the thickness, and the order of the shielding materials. This investigation looks at each of these problems and demonstrates how LASSO and Elastic Net respond to each. Four separate cases will be investigated: a shielded and unshielded masking and convoluted example. For each, a high, medium, and low count trial will evaluate the effectiveness and limit to each method. The results will be evaluated based on the prediction accuracy using 20 separate runs.
5.2 Masking Without Shielding

To replicate an ideal masking situation, a small Co-57 contribution was included to a spectrum with Ba-133, Na-22, and Cs-137. Table 5-1 provides the coefficients used in the generation of
the simulated combination spectrum. Each combination spectrum consists of the library output from MCNP multiplied by the linear coefficient, added to each library used in the combination spectrum, and given random Poisson distributed noise. Figures 5-3 thru 5-8 show a random fit for a low, medium, and high count rate for both LASSO and Elastic Net. Table 5-2 displays the accuracy at predicting the correct components to the model.

<table>
<thead>
<tr>
<th>Table 5-1: Masking coefficients and total counts</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Masking Linear Coefficients</strong></td>
</tr>
<tr>
<td><strong>Ba-133</strong></td>
</tr>
<tr>
<td><strong>Na-22</strong></td>
</tr>
<tr>
<td><strong>Mn-54</strong></td>
</tr>
<tr>
<td><strong>Cs-137</strong></td>
</tr>
<tr>
<td><strong>Co-60</strong></td>
</tr>
<tr>
<td><strong>Co-57</strong></td>
</tr>
<tr>
<td><strong>Total Counts</strong></td>
</tr>
</tbody>
</table>

Figure 5-3: LASSO masking low count rate fit
Figure 5-4: Elastic Net masking low count rate fit

Figure 5-5: LASSO masking medium count rate fit
Figure 5-6: Elastic Net masking medium count rate fit

Figure 5-7: LASSO masking high count rate fit
Figure 5-8: Elastic Net masking high count rate fit

Table 5-2: Masking trial prediction accuracy for LASSO and Elastic Net with varying count rates

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ba-133</strong></td>
<td>0.85</td>
<td>0.65</td>
<td>0.95</td>
<td>0.75</td>
<td>1.00</td>
<td>0.85</td>
</tr>
<tr>
<td><strong>Na-22</strong></td>
<td>0.95</td>
<td>0.90</td>
<td>1.00</td>
<td>0.95</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td><strong>Mn-54</strong></td>
<td>0.65</td>
<td>0.60</td>
<td>0.55</td>
<td>0.55</td>
<td>0.75</td>
<td>0.50</td>
</tr>
<tr>
<td><strong>Cs-137</strong></td>
<td>0.95</td>
<td>0.75</td>
<td>1.00</td>
<td>0.90</td>
<td>1.00</td>
<td>0.85</td>
</tr>
<tr>
<td><strong>Co-60</strong></td>
<td>0.55</td>
<td>0.40</td>
<td>0.60</td>
<td>0.75</td>
<td>0.75</td>
<td>0.70</td>
</tr>
<tr>
<td><strong>Co-57</strong></td>
<td>0.40</td>
<td>0.35</td>
<td>0.50</td>
<td>0.30</td>
<td>0.70</td>
<td>0.40</td>
</tr>
</tbody>
</table>

The results demonstrate that LASSO is far more effective at correctly selecting the correct model. As the count rate is increased, LASSO demonstrates an ability to detect even small contributions of Co-57 at a 70% rate, while only having a false positive rate of 25%.
5.3 Convolution Without Shielding

To replicate an ideal convolution situation, contributions of both Na-22 and Co-60 are used. Table 5-3 provides the coefficients used in the generation of the simulated combination spectrum. Each combination spectrum consists of the library output from MCNP multiplied by the linear coefficient, added to each library used in the combination spectrum, and given random Poisson distributed noise. Figures 5-9 thru 5-14 show a random fit for a low, medium, and high count rate for both LASSO and Elastic Net. Table 5-4 displays the accuracy at predicting the correct components to the model.

**Table 5-3: Convolution coefficients and total counts**

<table>
<thead>
<tr>
<th>Convolution Linear Coefficients</th>
<th>Ba-133</th>
<th>Na-22</th>
<th>Mn-54</th>
<th>Cs-137</th>
<th>Co-60</th>
<th>Co-57</th>
<th>Total Counts</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>125,000</td>
<td>0</td>
<td>20,000</td>
<td>200,000</td>
<td>5,000</td>
<td>4,817</td>
</tr>
<tr>
<td>0</td>
<td>2,000,000</td>
<td>2,000,000</td>
<td>0</td>
<td>1,000,000</td>
<td>50,000</td>
<td>64,407</td>
<td>646,974</td>
</tr>
<tr>
<td>0</td>
<td>20,000,000</td>
<td>20,000,000</td>
<td>0</td>
<td>10,000,000</td>
<td>500,000</td>
<td>646,974</td>
<td></td>
</tr>
</tbody>
</table>
**Figure 5-9:** LASSO convolution low count rate fit

**Figure 5-10:** Elastic Net convolution low count rate fit
Figure 5-11: LASSO convolution medium count rate fit

Figure 5-12: Elastic Net convolution medium count rate fit
Figure 5-13: LASSO convolution high count rate fit

Figure 5-14: Elastic Net convolution high count rate fit
Table 5-4: Convolution trial prediction accuracy for LASSO and Elastic Net with varying count rates

<table>
<thead>
<tr>
<th></th>
<th>Convolution Without Shielding Prediction Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba-133</td>
<td>0.90</td>
</tr>
<tr>
<td>Na-22</td>
<td>1.00</td>
</tr>
<tr>
<td>Mn-54</td>
<td>0.75</td>
</tr>
<tr>
<td>Cs-137</td>
<td>0.85</td>
</tr>
<tr>
<td>Co-60</td>
<td>1.00</td>
</tr>
<tr>
<td>Co-57</td>
<td>0.15</td>
</tr>
</tbody>
</table>

The results demonstrate that LASSO is far more effective at accurately selecting the correct model for the convolved peak application. As the count rate is increased, LASSO demonstrates an ability to decipher contributions of both Co-60 and Na-22 at 100% rate, while only having a false positive rate of 35%. Co-57 has a minor contribution to the overall spectrum and with the highest prediction rate of 60%, this demonstrates that the contribution may be close to the detectable limit for these methods.

5.4 Masking with Shielding

To perform the masking with shielding problem, the same steps from section 5.2 were taken. In order to create a different response, shielded libraries using 1 inch of aluminum placed half way between the detector and source were used to create the combination spectrum. Table 5-5 provides the coefficients used in the generation of the simulated combination spectrum. Figures 5-15 thru 5-20 show a random fit for a low, medium, and high count rate for both LASSO and Elastic Net. Table 5-6 displays the accuracy at predicting the correct components to the model.
### Table 5-5: Masking with Shielding coefficients and total counts

<table>
<thead>
<tr>
<th></th>
<th>Masking with Shielding Linear Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ba-133</strong></td>
<td>30,000</td>
</tr>
<tr>
<td><strong>Na-22</strong></td>
<td>100,000</td>
</tr>
<tr>
<td><strong>Mn-54</strong></td>
<td>0</td>
</tr>
<tr>
<td><strong>Cs-137</strong></td>
<td>100,000</td>
</tr>
<tr>
<td><strong>Co-60</strong></td>
<td>0</td>
</tr>
<tr>
<td><strong>Co-57</strong></td>
<td>5,000</td>
</tr>
<tr>
<td><strong>Total Counts</strong></td>
<td>4956</td>
</tr>
</tbody>
</table>

**Figure 5-15:** LASSO masking with shielding low count rate fit
Figure 5-16: Elastic Net masking with shielding low count rate fit

Figure 5-17: LASSO masking with shielding medium count rate fit
**Figure 5-18:** Elastic Net masking with shielding medium count rate fit

**Figure 5-19:** LASSO masking with shielding high count rate fit
The results demonstrate that LASSO is far more effective at correctly selecting the correct model. As the count rate is increased, LASSO demonstrates an ability to detect even small contributions of Co-57 at a 55% rate, while only having a false positive rate of 30%.

### 5.5 Convolution with Shielding

To replicate an ideal convolution with shielding situation the same steps from section 5.3 were taken. In order to create a different response, shielded libraries using 1 inch of aluminum placed halfway between the detector and source were used to create the combination spectrum. Table 5-
7 provides the coefficients used in the generation of the simulated combination spectrum. Figures 5-21 thru 5-26 show a random fit for a low, medium, and high count rate for both LASSO and Elastic Net. Table 5-8 displays the accuracy at predicting the correct components to the model.

**Table 5-7: Convolution with shielding coefficients and total counts**

<table>
<thead>
<tr>
<th></th>
<th>Convolution with Shielding Linear Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ba-133</strong></td>
<td>0 0 0</td>
</tr>
<tr>
<td><strong>Na-22</strong></td>
<td>125,000 2,000,000 20,000,000</td>
</tr>
<tr>
<td><strong>Mn-54</strong></td>
<td>0 0 0</td>
</tr>
<tr>
<td><strong>Cs-137</strong></td>
<td>20,000 200,000 2,000,000</td>
</tr>
<tr>
<td><strong>Co-60</strong></td>
<td>100,000 1,000,000 10,000,000</td>
</tr>
<tr>
<td><strong>Co-57</strong></td>
<td>5,000 50,000 500,000</td>
</tr>
<tr>
<td><strong>Total Counts</strong></td>
<td>4,387 61,327 61,756</td>
</tr>
</tbody>
</table>

**Figure 5-21:** LASSO convolution with shielding low count rate fit
Figure 5-22: Elastic Net convolution with shielding low count rate fit

Figure 5-23: LASSO convolution with shielding medium count rate fit
**Figure 5-24:** Elastic Net convolution with shielding medium count rate fit

**Figure 5-25:** LASSO convolution with shielding high count rate fit
Figure 5-26: Elastic Net convolution with shielding high count rate fit

Table 5-8: Convolution with shielding trial prediction accuracy for LASSO and Elastic Net with varying count rates

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba-133</td>
<td>0.65</td>
<td>0.70</td>
<td>0.65</td>
<td>0.90</td>
<td>0.60</td>
<td>0.75</td>
</tr>
<tr>
<td>Na-22</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Mn-54</td>
<td>0.70</td>
<td>0.60</td>
<td>0.50</td>
<td>0.45</td>
<td>0.50</td>
<td>0.50</td>
</tr>
<tr>
<td>Cs-137</td>
<td>0.70</td>
<td>0.80</td>
<td>1.00</td>
<td>0.95</td>
<td>0.95</td>
<td>1.00</td>
</tr>
<tr>
<td>Co-60</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Co-57</td>
<td>0.40</td>
<td>0.50</td>
<td>0.70</td>
<td>0.65</td>
<td>0.60</td>
<td>0.80</td>
</tr>
</tbody>
</table>

The results demonstrate that each method is effective at accurately selecting the correct model for the convolved peak application. As the count rate is increased, LASSO and Elastic Net demonstrate an ability to decipher contributions of both Co-60 and Na-22 at 100% rate, with a false positive rate of 50%.
CHAPTER 6

Discussion and Conclusions

This dissertation takes a deep look into supervised machine learning variable selection techniques, LASSO and Elastic Net, and their use in advancing nuclear security related technologies. Oil well logging tools provide a soft target opportunity for bad characters to steal radioactive material for use in a dirty bomb. Using a D-T pulsed neutron generator and a digitizer, prompt and delayed detector responses can be obtained, providing a real time background suppression technique. With the background suppressed, it becomes possible to use LASSO and Elastic Net on-line for a real time analysis technique. LASSO and Elastic Net both show promise in the oil well logging application, with LASSO performing slightly better overall.

Several improvements can be made to the overall experiment moving forward. NaI scintillation detectors were used. More modern detectors, such as LaBr or CeBr offer a faster response time, improved resolution, and a higher density. Each of these properties will impact the overall count rate and distinct features for each code to interpret. Additionally, no measures were taken to accurately determine the make up of each of the materials. The research group at Kansas State University provided experimental data with labels of water, limestone, or sand with no additional information. Concentration values of different elements in each of these materials varies widely, as well as other characteristics such as density and porosity. An in-depth chemical analysis in the future would serve as a basis to truly determine the effectiveness of the variable selection and final fits.

Prior to the completion of this dissertation, several oil industry experts mentioned the need to improve cross sectional data for calcium. Some of the fitting issues with the limestone measurement can be attributed to poor cross-sectional data being fed into the simulations. Oil well companies correct the differences using semi-empirical fits that the North Carolina State research group does not have access to.
LASSO and Elastic Net were also used to aim to improve on existing handheld radioisotope identification devices (RIIDs) used by first responders in field applications. Current RIID algorithms have difficulty in situations where clean peaks are not present such as masking and convolved peak cases. Once again, LASSO outperformed Elastic Net in almost every test run. As the count rate increased, the overall effectiveness of each method improved significantly. Even low concentrations of Co-57 were able to be detected at a rate greater than 50%.

Moving forward, LASSO should be considered for use in any radiation detection application that can be solved with linear methods. Elastic Net should also be considered for any application where there is high correlation between data. These methods have been demonstrated to be effective at correctly identifying model parameters that can improve the efficiency of oil well logging operators, potentially saving money and providing incentive to switch to the use of pulsed neutron generators.
REFERENCES


MCNP Training Manual


APPENDICES
Appendix A: MCNP Sample Deck – KSU Application

Room 207 - Salt Water simulation

c

c --------- Cell Cards

c Detectors
20  37  -0.00276  -30  imp:n,p=1  $ BF-3 detector 1
21  39  -3.67    -31  imp:n,p=1  $ NaI detector 1
22  38  -0.2677  -32  imp:n,p=1  $ Helium-3 detector 2
23  39  -3.67   -33  imp:n,p=1  $ NaI detector 2
24  30  -11.34   -34  imp:n,p=1  $ Lead Shield, 2 inches
130  6  -0.998207  -115 118 -230 113  imp:n,p=1  $ inside Shell 1
131  6  -0.998207  -115 230 -231 113  imp:n,p=1  $ inside Shell 2
132  6  -0.998207  -115 231 -232 113  imp:n,p=1  $ inside Shell 3
133  6  -0.998207  -115 232 -233 113  imp:n,p=1  $ inside Shell 4
134  6  -0.998207  -115 233 -234 113  imp:n,p=1  $ inside Shell 5

c BEE chamber
105  0  -40 114 116 113 120  imp:n,p=1  $ room air
106  1  -2.35  40 -41 101 102 103 110 111 112 113 114  imp:n,p=1  $ room walls
107  1  -2.35  -116 115 118  imp:n,p=1  $ BEE walls
108  6  -0.998207  -115 234 113  imp:n,p=1  $ inside BEE
109  5  -2.7  -118 117  imp:n,p=1  $ borehole pipe
110  0  -117 119  #20 #21 #22 #23 #24  imp:n,p=1  $ inside borehole
99  0  41  -99 104 105 106 121  imp:n,p=1  $ void

c doors and door shields
120  0  -112  imp:n,p=1  $ inner door void
121  0  -110  imp:n,p=1  $ outer door void
122  0  -111  imp:n,p=1  $ outer door plug
123  3  -1.00  -113 118  imp:n,p=1  $ inner wall shield (12 in)
124  3  -1.00  -119  imp:n,p=1  $ inside borehole shield (11 in)
125  3  -1.00  -114  imp:n,p=1  $ inner door shield (2 in)
126  3  -1.00  -120  imp:n,p=1  $ outer door shield (2 in)
127  3  -1.00  -121  imp:n,p=1  $ top wall shield (5 in)
c roof voids and shields
31  0  -101  imp:n,p=1  $ roof void 1
32  0  -102  imp:n,p=1  $ roof void 2
33  0  -103  imp:n,p=1  $ roof void 3
34  3  -1.00  -104  imp:n,p=1  $ skylight 1 shield
35  3  -1.00  -105  imp:n,p=1  $ skylight 2 shield
36  3  -1.00  -106  imp:n,p=1  $ skylight 3 shield
100  0  99  imp:n,p=0  $ graveyard

c --------- Surface Cards

c -- detectors
30 rcc  -25.5  53.34  -12.7  15 0 0  1.9  $ BF3, OD 1.5"
31 rcc  -50.5  53.34  -12.7  7.5 0 0  3.81  $ NaI, OD 3"
<table>
<thead>
<tr>
<th>Code</th>
<th>Value1</th>
<th>Value2</th>
<th>Value3</th>
<th>Value4</th>
<th>Value5</th>
<th>Value6</th>
<th>Value7</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>-85.5</td>
<td>53.34</td>
<td>-12.7</td>
<td>15 0 0</td>
<td>1.9</td>
<td>He3, OD 1.5&quot;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>33</td>
<td>-110.5</td>
<td>53.34</td>
<td>-12.7</td>
<td>7.5 0 0</td>
<td>3.81</td>
<td>NaI, OD 3&quot;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>34</td>
<td>8.5</td>
<td>13.58</td>
<td>49.84</td>
<td>56.84</td>
<td>-16.2 -9.2</td>
<td>Pb Block</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>c -- Barriers</td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>-152.4</td>
<td>396.24</td>
<td>-426.72</td>
<td>152.4</td>
<td>193.04</td>
<td>$inside room</td>
<td></td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>-182.8</td>
<td>441.96</td>
<td>-457.20</td>
<td>182.88</td>
<td>-175.26</td>
<td>223.52 $outside room</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>c -- roof voids</td>
<td></td>
<td></td>
</tr>
<tr>
<td>101</td>
<td>-152.4</td>
<td>396.24</td>
<td>30.48</td>
<td>152.4</td>
<td>193.04</td>
<td>$skylight void 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>102</td>
<td>-152.4</td>
<td>396.24</td>
<td>-175.26</td>
<td>53.34</td>
<td>193.04</td>
<td>$skylight void 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>103</td>
<td>-152.4</td>
<td>396.24</td>
<td>-381.00</td>
<td>-259.08</td>
<td>193.04</td>
<td>$skylight void 3</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>c -- roof shields</td>
<td></td>
<td></td>
</tr>
<tr>
<td>104</td>
<td>-167.6</td>
<td>411.48</td>
<td>15.24</td>
<td>167.64</td>
<td>223.52</td>
<td>$6&quot; poly over 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>105</td>
<td>-167.6</td>
<td>411.48</td>
<td>-190.5</td>
<td>-38.1</td>
<td>223.52</td>
<td>$6&quot; poly over 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>106</td>
<td>-167.6</td>
<td>411.48</td>
<td>-396.24</td>
<td>-243.84</td>
<td>223.52</td>
<td>$6&quot; poly over 3</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>c -- doors and door shields</td>
<td></td>
<td></td>
</tr>
<tr>
<td>110</td>
<td>421.64</td>
<td>441.96</td>
<td>-188.54</td>
<td>-85.72</td>
<td>99.06</td>
<td>$outer door void</td>
<td></td>
<td></td>
</tr>
<tr>
<td>111</td>
<td>396.24</td>
<td>421.64</td>
<td>-188.54</td>
<td>-85.72</td>
<td>99.06</td>
<td>$outer door plug</td>
<td></td>
<td></td>
</tr>
<tr>
<td>112</td>
<td>-182.8</td>
<td>-152.4</td>
<td>-188.54</td>
<td>-85.72</td>
<td>99.06</td>
<td>$inner door void</td>
<td></td>
<td></td>
</tr>
<tr>
<td>113</td>
<td>-152.4</td>
<td>121.92</td>
<td>7.62</td>
<td>99.06</td>
<td>114.30</td>
<td>$inner wall shield</td>
<td></td>
<td></td>
</tr>
<tr>
<td>114</td>
<td>-152.4</td>
<td>147.32</td>
<td>-198.12</td>
<td>-76.20</td>
<td>114.30</td>
<td>$inner door shield</td>
<td></td>
<td></td>
</tr>
<tr>
<td>120</td>
<td>391.16</td>
<td>396.24</td>
<td>-198.12</td>
<td>-76.20</td>
<td>114.30</td>
<td>$outer door shield</td>
<td></td>
<td></td>
</tr>
<tr>
<td>121</td>
<td>-35.56</td>
<td>86.36</td>
<td>182.88</td>
<td>195.58</td>
<td>114.30</td>
<td>$top wall shield</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>c -- enclosure walls</td>
<td></td>
<td></td>
</tr>
<tr>
<td>115</td>
<td>-152.4</td>
<td>91.44</td>
<td>-45.72</td>
<td>152.4</td>
<td>114.30</td>
<td>$inside BEE walls</td>
<td></td>
<td></td>
</tr>
<tr>
<td>116</td>
<td>-152.4</td>
<td>111.76</td>
<td>-66.04</td>
<td>152.4</td>
<td>114.30</td>
<td>$outside BEE walls</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>c -- borehole pipe</td>
<td></td>
<td></td>
</tr>
<tr>
<td>117</td>
<td>-152.4</td>
<td>53.34</td>
<td>-12.7</td>
<td>264.16</td>
<td>0 0</td>
<td>$inside borehole</td>
<td></td>
<td></td>
</tr>
<tr>
<td>118</td>
<td>-152.4</td>
<td>53.34</td>
<td>-12.7</td>
<td>264.16</td>
<td>0 0</td>
<td>$outside borehole</td>
<td></td>
<td></td>
</tr>
<tr>
<td>119</td>
<td>-152.4</td>
<td>53.34</td>
<td>-12.7</td>
<td>27.94</td>
<td>0 0</td>
<td>$shielding inside borehole</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>99 SO 800 $problem boundary</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>c -- tally surfaces</td>
<td></td>
<td></td>
</tr>
<tr>
<td>230</td>
<td>C/X</td>
<td>53.34</td>
<td>-12.7</td>
<td>20.80</td>
<td>$Shell 1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>231</td>
<td>C/X</td>
<td>53.34</td>
<td>-12.7</td>
<td>30.80</td>
<td>$Shell 2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>232</td>
<td>C/X</td>
<td>53.34</td>
<td>-12.7</td>
<td>40.80</td>
<td>$Shell 3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>233</td>
<td>C/X</td>
<td>53.34</td>
<td>-12.7</td>
<td>50.80</td>
<td>$Shell 4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>234</td>
<td>C/X</td>
<td>53.34</td>
<td>-12.7</td>
<td>60.80</td>
<td>$Shell 5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>c -------- DATA CARDS</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>SDEF par=n erg=14 POS 25.4 53.34 -12.7 WGT=12653259</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>ACT FISSION=none NONFISS=ALL</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>PHYS:N 6j 3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>PHYS:p 100 0 0 0 0</td>
<td>j 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>CUT:N 2j 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>c</td>
<td>c ctme 4400</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
nps 50000000
mode n p
c
c --- NEUTRON TALLIES
f12:n 118.1 230 231 232 233 234
sd12 14478 27884 41289 54695 68101 81507
f22:n 118.1 230 231 232 233 234
sd22 1 1 1 1 1 1
c --- BF3 Near
f28:N 20
E28 0 2046i 10
c --- He3 Far
f38:N 22
E38 0 2046i 10
c --- NaI Near
f68:P 21
E68 0 2046i 10
c --- NaI Far
f78:P 23
E78 0 2046i 10
c
c ------------------------------------------
c    NBS Concrete (density = 2.35 g/cm^3)
c ------------------------------------------
m1  1001.60c -0.0056  $ hydrogen
    16032.60c -0.0012  $ sulfur
    8016.60c -0.4983  $ oxygen
    14000.60c -0.3158  $ silicon
    13027.60c -0.0456  $ aluminum
    26000.55c -0.0122  $ iron
    20000.60c -0.0826  $ calcium
    19000.60c -0.0192  $ potassium
    11023.60c -0.0171  $ sodium
    12000.60c -0.0024  $ magnesium
c
c ************************************************************
c    AIR: ANSI/ANS-6.4.3, Dry air; density = 0.0012 g/cm^3
c          Composition by mass fraction
 ************************************************************
m2   7014.60c  -.75519
    8016.60c  -.23179
    6000.60c  -.00014
    18000.35c  -.01288
c
c --------------------------------------------------------------------
c       material: borated polyethylene d=1.00 g/cm^3  CH2 + 8 wt% B4C
B-11 5.029; B-10 1.234; C 80.595; H 13.143

m3 1001.60c -0.13143
    5010.60c -0.01234
    5011.60c -0.05029
    6000.60c -0.80594


material: polyethylene d=0.95 g/cm^3  CH2

m4 1001.60c 2
    6000.60c 1

material: aluminum 6061; density=2.7 g/cm^3

m5 12000 -0.01000 $ Mg
    13027 -0.97200 $ Al
    14000 -0.00600 $ Si
    22000 -0.00088 $ Ti
    24000 -0.00195 $ Cr
    25055 -0.00088 $ Mn
    26000 -0.00409 $ Fe
    29000 -0.00275 $ Cu
    30000 -0.00146 $ Zn

water; density = 0.998207 g/cm^3

m6 1001.60c 2
    8016.60c 1

salt water, 0.9%; density = 1.00875 g/cm^3

m7 1001.60c -0.1101992
    8016.60c -0.8801130
    11023.60c -0.0035084
    17035.70c -0.0041186
    17037.70c -0.0013729

salt water, 1.8%; density = 1.00875 g/cm^3

m8 1001.60c -0.1091984
    8016.60c -0.8721200
    11023.60c -0.0070168
    17035.70c -0.0082372
    17037.70c -0.0027458
c salt water, 2.7%; density = 1.00875 g/cm^3

c ---
m9  1001.60c  -0.1081111
   8016.60c  -0.8648888
   11023.60c -0.0105252
   17035.70c -0.0123561
   17037.70c -0.0041187

c salt water, 3.6%; density = 1.00875 g/cm^3

c ---
m10 1001.60c  -0.1071111
   8016.60c  -0.8568888
   11023.60c -0.0140339
   17035.70c -0.0164746
   17037.70c -0.0054915

c Sodium; density -0.97

c ---
m11 11000 -0.97

c Chlorine; density -1.5625

c ---
m12 17000 -1.5625

c ---- Lead, Inert: Density (11.34 g/cm^3)
m30  82000 -1.000000 $ He

c ---- BF-3, Proportional: Density (0.00276 g/cm^3)
m37  5000  1 $ B
   9000  3 $ F

c ---- Helium-3, Proportional: Density (0.2677 g/cm^3)
m38  2003 -1.000000 $ He

c -------- Nal Crystal: Density (3.67 g/cm^3)
m39  11023.60c  0.500 $ Na
   53127  0.500 $ I

c -------- Nickel Additive: Density (8.908 g/cm^3)
m40  28058.60c -0.68077
   28060.60c -0.26223
   28061.60c -0.01139
   28062.60c -0.03635
   28064.60c -0.00926
import pandas as pd
import numpy as np
from numpy import array
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import scale
from sklearn.linear_model import Lasso, LassoCV
from sklearn.metrics import mean_squared_error

libraries = pd.read_csv("NearExplibraries.csv")
target = pd.read_csv("waternearinterp.csv")
energy = pd.read_csv("Energy.csv")

X = libraries[200:1500]
y = target.y[200:1500]
originalenergy = energy[200:1500]

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=.90)
alphas = 10**np.linspace(6,-2,1000)*.5
lassocv = LassoCV(alphas=None, cv=10, max_iter=100000, normalize=True, positive=False)
model = lassocv.fit(X_train, y_train)

m_log_alphas = -np.log10(model.alphas_)
plt.figure()
plt.plot(m_log_alphas, np.log10(model.mse_path_), ':')
plt.plot(m_log_alphas, np.log10(model.mse_path_.mean(axis=-1)), 'k', label='Average across the folds', linewidth=2)
plt.axvline(-np.log10(model.alpha_), linestyle='--', color='k', label='alpha: CV estimate')
plt.legend()
plt.xlabel('-log(alpha)')
plt.ylabel('Mean square error')
plt.title('Mean square error on each fold: coordinate descent')
plt.axis('tight')
plt.show()

lasso = Lasso(max_iter=10000, normalize=True, positive=True)
coefs = []

for a in alphas:
lasso.set_params(alpha=a)
lasso.fit(scale(X_train), y_train)
coefs.append(lasso.coef_)

label_list=['Sand Near', 'Water Near', 'Limestone Near', 'Iron', 'Copper']
ax = plt.gca()
lineObjects = ax.plot(alphas*2, coefs)
ax.set_yscale('log')
plt.ticklabel_format(axis='y', style='sci', scilimits=(0,0))
plt.locator_params(axis='y', nbins=10)

plt.xlabel('Alpha')
plt.ylabel('Coefficients')
plt.axvline(model.alpha_, linestyle='--', color='k',label='alpha: CV estimate')
plt.title('Optimal Alpha Parameters')
plt.legend(iter(lineObjects), label_list)
plt.show()

lasso.set_params(alpha=lassocv.alpha_)
lasso.fit(X_train, y_train)
mean_squared_error(y_test, lasso.predict(X_test))
print("Best for alphas:")
print(lassocv.alpha_)

print("Best l1-ratio:")
print(lasso.l1_ratio)

print("Coefficients:")
print(pd.Series(lasso.coef_, index=X.columns))
print(mean_squared_error(y_test, lasso.predict(X_test)))
fit = lasso.coef_*X
total = lasso.coef_*libraries
full = total.Water_Near + total.Sand_Near + total.Limestone_Near + total.Iron + total.Copper

plt.semilogy(originalenergy, y, 'k', label='KSU Experimental Data')
plt.semilogy(originalenergy, fit.Water_Near, label='Water Library')
plt.semilogy(originalenergy, fit.Sand_Near, label='Sand Library')
plt.semilogy(originalenergy, fit.Limestone_Near, label='Limestone Library')
plt.semilogy(originalenergy, fit.Iron, label='Iron Library')
plt.semilogy(originalenergy, fit.Copper, label='Copper Library')
plt.semilogy(originalenergy, comb, label='Fit')
plt.legend()
plt.xlabel('Energy (MeV)')
plt.ylabel('Counts')
plt.title('LASSO Library Fit')
plt.show()

plt.semilogy(energy, target.y, 'k', label='KSU Experimental Data')
plt.semilogy(energy, total.Water_Near, label='Water Near Library')
plt.semilogy(energy, total.Sand_Near, label='Sand Near Library')
plt.semilogy(energy, total.Limestone_Near, label='Limestone Near Library')
plt.semilogy(energy, total.Iron, label='Iron Library')
plt.semilogy(energy, total.Copper, label='Copper Library')
plt.semilogy(energy, full, label='Fit')

plt.legend()
plt.xlabel('Energy (MeV)')
plt.ylabel('Counts')
plt.title('LASSO Library Fit')
plt.show()
Appendix C: Elastic Net Code Sample

```python
import pandas as pd
import numpy as np
from numpy import array
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import scale
from sklearn.linear_model import Lasso, LassoCV, ElasticNet, ElasticNetCV,
lasso_path, enet_path
from sklearn.metrics import mean_squared_error
import pylab as pl

libraries = pd.read_csv("NearExplibraries.csv")
target = pd.read_csv("waternearinterp.csv")
energy = pd.read_csv("Energy.csv")

X = libraries[200:1500]
y = target.y[200:1500]
originalenergy = energy[200:1500]

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=.90)
coefs = []
alphas = 10**np.linspace(10,-2,100)*.5

ten = ElasticNetCV(l1_ratio=.99, alphas=None, cv=10, max_iter=100000,
normalize=True, positive=True)
ten.fit(X_train, y_train)
ElasticNet = ElasticNet(l1_ratio=.99,max_iter=10000, normalize=True, positive=True)
# Display results
model = en.fit(X_train, y_train)
m_log_alphas = -np.log10(model.alphas_)

plt.figure()
plt.plot(m_log_alphas, np.log10(model.mse_path_), ':')
plt.plot(m_log_alphas, np.log10(model.mse_path_.mean(axis=-1)), 'k', label='Average
across the folds', linewidth=2)
plt.axvline(-np.log10(model.alpha_), linestyle='--', color='k', label='alpha: CV estimate')
plt.legend()
plt.xlabel('-log(alpha)')
plt.ylabel('Mean square error')
plt.title('Mean square error on each fold: coordinate descent')
plt.axis('tight')
plt.show()
```
for a in alphas:
    ElasticNet.set_params(alpha=a)
    ElasticNet.fit(scale(X_train), y_train)
    coefs.append(ElasticNet.coef_)

label_list=['Sand Library', 'Water Library', 'Limestone Library', 'Iron Library', 'Copper Library']
ax = plt.gca()
lineObjects = ax.plot(alphas, coefs)
ax.set_xscale('log')
plt.ticklabel_format(axis='y', style='sci', scilimits=(0,0))
plt.axvline(en.alpha_, linestyle='--', color='k', label='alpha: CV estimate')
plt.locator_params(axis='y', nbins=10)

plt.xlabel('Alpha')
plt.ylabel('Coefficients')
plt.title('Optimal Alpha Parameters')
plt.legend(iter(lineObjects), label_list)
plt.show()
print("Best for alphas:")
print(en.alpha_)
print("Best L1-ratio:")
print(en.l1_ratio_)
print("Coefficients:")
print(pd.Series(en.coef_, index=X.columns))

#evaluate
y_pred = en.predict(X_test)
test_score = mean_squared_error(y_test, y_pred)
print(test_score)

fit = en.coef_*X
total = en.coef_*libraries
full = total.Water_Near + total.Sand_Near + total.Limestone_Near + total.Iron +
total.Copper

plt.semilogy(originalenergy, y, 'k', label='KSU Experimental Data')
plt.semilogy(originalenergy, fit.Water_Near, label='Water Library')
plt.semilogy(originalenergy, fit.Sand_Near, label='Sand Library')
plt.semilogy(originalenergy, fit.Limestone_Near, label='Limestone Library')
plt.semilogy(originalenergy, fit.Iron, label='Iron Library')
plt.semilogy(originalenergy, fit.Copper, label='Copper Library')