Deep Learning for Germanium-Based Neutrinoless Double-Beta Decay Searches

Julieta Gruszko NP AI/ML PI Exchange Meeting November 30, 2022



THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL









Outline



- Double-Beta Decay in ⁷⁶Ge
- Interpretable BDT
- Semi-Autonomous Data Cleaning
- Electronics Response Modeling
- Other Projects & Details







Why Neutrinoless Double Beta Decay?

- The discovery of $0\nu\beta\beta$ decay would dramatically revise our foundational understanding of physics and the cosmos
 - Lepton number is not conserved
 - The neutrino is a fundamental Majorana particle
 - There is a potential path for understanding the matter antimatter asymmetry in the cosmos, through leptogenesis
 - There is a new mechanism demonstrated for the generation of mass

- The search for $0\nu\beta\beta$ decay is one of the most compelling and exciting challenges in all of contemporary physics
- The LEGEND Collaboration aspires to meet this challenge through a ton-scale search for $0\nu\beta\beta$ decay of ^{76}Ge

Designing for Unambiguous Discovery

- What is required for a discovery of 0vββ decay?
- Long half-lives mean you need large exposures. For 3-4 counts of 0vββ at...
 - 10²⁶ years: 100 kg-years
 - 10²⁷ years: 1 ton-year
 - 10²⁸ years: 10 ton-years
- Need a good signal-to-background ratio to get statistical significance
 - A very low background event rate
 - The best possible energy resolution

Simulated LEGEND-1000 example spectrum for $T_{1/2} = 10^{28}$ yrs, BI < 10⁻⁵ cts/keV kg yr, after cuts, from 10 years of data



At every stage, 0vββ searches in ⁷⁶Ge are designed for unambiguous discovery: their goal is quasi-background free operation for their full exposure

Backgrounds and Discovery

- Background-free: Sensitivity rises linearly with exposure Background-limited: Sensitivity rises as the square root of exposure
- Our background goal is "quasi-background-free" operation
 - Less than one background count expected in a 4σ Region of Interest (ROI) with the full exposure (FWHM: Full Width at Half Maximum; 2.355 σ for a Gaussian peak)



Germanium Detector Innovation



Materials from the GERDA and MAJORANA Collaborations

Background Rejection in Point Contact Detectors

Ovββ signal candidate (single-site)



γ-background (multi-site)



External α, β, and γ backgrounds all create distinctive pulse shapes, allowing for highly efficient ββ decay event selection

Surface background on n+ contact



Surface background on p+ contact



Energy and Pulse Shape Parameter Calibration



- Weekly Th-228 source deployments used for energy scale calibration
- Also used for pulse shape discrimination parameter calibration
 - Double Escape Peak: single-site 0vββ proxy
 - Single Escape Peak: multi-site proxy



From the Current Generation to the Ton Scale



MJD: Final $0\nu\beta\beta$ results in review

arXiv: 2207.07638 (2022)



GERDA: Final $0\nu\beta\beta$ results published





LEGEND-200: Now in commissioning



LEGEND-1000: Conceptual design development continuing

arXiv: 2107.11462

Implications for AI/ML

- Granular Detectors + Low Backgrounds
 - \rightarrow Low rate of physics events (< 1 Hz per detector)
 - ightarrow Noise-induced events can make up a large fraction of triggered waveforms
 - \rightarrow Allows time-intensive analysis of final waveforms, but algorithms should also run on much larger calibration data sets to confirm signal acceptance rate and stability
- "Traditional" pulse-shape parameters perform quite well for background rejection
 - ightarrow Build network structures that improve on existing pulse-shape parameters
 - ightarrow Use AI/ML for tasks other than signal/background event classification
- Discovery could be claimed based on as few as 3 events
 → Analysis interpretability is key

Project Goals

- Overall goal: improve scalability and capabilities of analysis methods for the Majorana Demonstrator and LEGEND using ML tools
- 5 projects within these goals:
 - Interpretable Boosted Decision Tree for MJD and LEGEND
 - Semi-autonomous Data Cleaning for LEGEND-200
 - Electronics Response Emulation and Removal for LEGEND
 - Self-supervised Learning for Waveform Classification in LEGEND
 - Build Local High-Powered Computer for Algorithm Prototyping

Interpretable Boosted Decision Tree



Due to charge trapping and charge cloud diffusion in the detector bulk, traditional analysis parameters are often highly correlated: standard analysis fits the largest linear bi-variate correlations detector-by-detector and corrects for them

BDT method developed to...

- Utilize all the correlations to improve background reduction
- Reduce the need for additional targeted cuts like LQ
- Develop method for future experiments like LEGEND
 - Reduce need for detector-by-detector calibration
 - Reduce need for run-by-run calibration
 - Address increased correlations in larger-mass detectors
- Leverage interpretability to learn from the machine



Boosted Decision Tree

O Decision tree is highly interpretable model

O Boosting algorithm utilizes ensemble learning to makes it **powerful**

O Naturally handle categorical features and continuous features together



- Leverages pre-existing pulse shape parameters
- We train 2 BDTs based on a labeled training data sample from MJD: MSBDT and α BDT

LightGBM

Data Selection, Augmentation, and Distribution Matching

• Signal: the DEP events from calibration

1,738 genuine α are collected in total

DCR

Background: Collecting a events from low background

High energy: above 2615keV single site events

Low energy: 1000-2615keV events failing the DCR cut

aBDT:

runs:

•

AVSE



MultisiteBDT:

ISENRICHED

- Training on weekly ²²⁸Th calibration dataset
- Collect single escape peak (SEP) and double escape peak (DEP) by energy cut

DETECTOR

~100,000 events per peak

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DRIFT TIME



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NOISE

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Data Augmentation:

- Perform SMOTE-NC to boost the training α population
 - Linear interpolation for continuous feature
 - Majority vote for categorical feature
- 1,738 genuine a → ~100,000 fake a
- Train aBDT using DEP vs. fake a

Distribution matching performed for "nonprimary" features

BDT Performance in MJD Data

Output(a.u.) 00000 00000

MSBDT:



Signal

Background



......

Classifier

BDT

Raw AvsE

DEP

Standard AvsE 89.6%±0.07%

89.6%±0.07%

89.8%±0.07%

SEP

5.71%±0.03%

6.25%±0.03%

7.40%±0.04%

1.000

0.975

0.950

True Positive Rate 0.900 0.900 0.875

0.850

0.825

αBDT:

BDT Performance in MJD



- Difference driven by late addition of LQ analysis parameter, which was not included in BDT
- Comparable result with far fewer person-hours! No detector-by-detector or run-by-run secondary calibration needed.
- Results accepted for publication in Phys. Rev. C, arXiv:2207.10710

BDT Interpretability



- Shapley value allows for feature importance analysis and event-by-event interpretability ۲
- Shows that BDT has "discovered" understood correlation of AvsE and drift time •
- Feeds back to improve traditional analysis: choose between similar parameters based ۲ on importance and implement new PSD based where BDT-outperforms
- Now being applied to LEGEND data and exploring the use of lower-level parameters

Julieta

tDrift50 tDrift

250

200

100

-50

0

50

100 Time [ns]

Sample α waveform

150

Semi-Autonomous Data Cleaning



Motivation

Advantages over traditional data cleaning:

- Adapts to changing run conditions
- Allows ID of new populations during commissioning
- Flexible framework can be used for detector characterization measurements in addition to LEGEND-200
- Could improve separability by using more waveform information



Unsupervised learning = **no labels** prior to training Supervised learning = **labels available** prior to training

Information Extraction



- Time-sensitive Fourier transform
- Haar wavelets for decomposition
- We use the Approximate Coefficients (AC) to represent pulse shape information



Affinity Propagation



- Obtain exemplars from AC based on their pulse shape
- Algorithm is vastly memoryintensive, we use a subset of our data to train

- Unsupervised learning clustering algorithm based on a "messagepassing" method between data points
- Automatically computes number of clusters, and returns an "exemplar" from each cluster



Extending AP Results



 SVM draws a decision boundary between different clusters, which allows us to extend the algorithm to out-of-sample data points

- Supervised learning algorithm for classification
- Browse exemplars from AP and choose the ones containing physical events we want to keep



Results and Upcoming Work

- Separate networks trained for calibration and low-background data
- Salting with pristine events used to check survival efficiency: >99.99%
- ML-based data cleaning now in use for LEGEND-200 commissioning
- This tool has also been used for detector characterization stand data-cleaning
- Paper in preparation



Electronics Response Emulation



Motivation

- Pulse-shape simulations based on detector response are quite advanced, but are not being used regularly for background modeling due to difficulties in modeling electronics chain response
- Fitting-based approach for MJD proved unfeasible:
 - Requires highly-degenerate 12-parameter fit
 - Instability in electronics causes changes over time, requiring repeated fits
- Emulating electronics would allow for moreaccurate background modeling and potentially, direct waveform fitting
- Electronics deconvolution would improve performance of PSD



Positional U-Net + CycleGAN

- 1D U-Net chosen as model
- Added positional encoding maps inspired by Transformer model





- Difficulty lies in training: we have ensembles of data waveforms and simulated waveforms, but not the 1-to-1 matching between them
- We want the network to convert each input into the correct counterpart, not just some member of the ensemble
- Cycle-GAN provides a solution

Results and Upcoming Work

- Preliminary results are showing good performance
- Technical paper published as part of the NeurIPS 2022
 Workshop on Machine Learning in the Physical Sciences: "Ad-hoc Pulse Shape Simulation using Cyclic Positional U-Net"
 https://ml4physicalsciences.gith ub.io/2022/
- Now working to improve input pulse-shape simulations and conduct further performance studies
- In the future: validate with Compton scanner (known event position) data



Other Projects and Details

Other Projects

- Local-computer assembly:
 - Delayed due to chip shortages in 2020-2021, now underway
 - NERSC transition to Perlmutter allowed us to prototype on CORI GPUs during Y1
- Self-supervised network for waveform classification:
 - Network structure in place and being used as exploratory tool
 - Now considering how to best implement classifiers

Deliverables and Schedule

Year	2022 2023						2024 Personnel			
Quarter	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	
Dates	11/30/21 - 1/1/22	1/1/22-4/1/22	4/1/22 - 7/1/22	7/1/22 - 10/1/22	10/1/22 - 1/1/23	1/1/23 - 4/1/23	4/1/23 - 7/1/23	7/1/23 - 10/1/23	10/1/23 - 11/30/23	
Task 1a: BDT for MJD	Complete BDT framework	Write internal technical document	Complete interna technical review	l Submit and publish paper	1					Aobo Li
Task 1b: BDT for LEGEND			Begin BDT analysis of L-200 commissioning data	5) g Present early a results internally	Present results at APS DNP Meeting , Complete vinternal technical	Complete internal technical review , Incorporate into analysis chain.	Publish first LEGEND-200 results, including BDT analysis			Henry Nachman, Aobo Li
Task 2: Data Cleaning	Begin testing framework		Complete	Present early results, Incorporate into eanalysis (framework	Write technica	l Publish technica r paper				Esteban Leon
Task 3: Electronics Emulation			Begin framework	Write and publish		Publish physics paper using test data	Implement for analysis and pulse shape simulations	Provide recommendations for LEGEND-1000	Publish LEGEND- 200 background model, incorporating emulation	Aobo Li, Julieta Gruszko
Task 4: High-Powered Computer					Orde component:	r Receive s components	Complete assembly and setup.			Aobo Li, Julieta Gruszko, E. Leon
Task 5: Semi-/Self-Supervised Learning	l	Build network structure					Begin tests of SSL on pulse shape simulations	Integrate data driven and simulations-based networks	- 1 1	Esteban Leon, Aobo Li, Julieta Gruszko

	FY21 (\$k)	FY22 (\$k)	Totals (\$k)
Funds allocated	226	224	450
Actual costs to date	215	0	215



SOUTH DAKOTA MINES

Technische Universität Münche

The MAJORANA Collaboration



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The LEGEND Collaboration





LEGEND mission: "The collaboration aims to develop a phased, ⁷⁶Ge based double-beta decay experimental program with discovery potential at a half-life beyond 10²⁸ years, using existing resources as appropriate to expedite physics results."

Approx. 260 members, 50 institutions, 11 countries



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LEGEND,

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Extra Slides

LEGEND

Large Enriched Germanium Experiment for Neutrinoless ββ Decay



HPGe Detectors for $0\nu\beta\beta$

- Easily available material, enrichment, and detector production
- Highly efficient: >90% ⁷⁶Ge use, ~70% signal ulletefficiency after all cuts
- Easy operation: low operating voltage (< 5 kV) ulletand cryogenic requirements (77-90K)
- Many tools to reduce backgrounds ۲
 - Multiplicity, timing, active veto shielding
 - Pulse-shapes used for event topology discrimination _
 - Demonstrated lowest (GERDA) and 2nd lowest (MJD) backgrounds
- Solid basis for unambiguous discovery
 - Superb energy resolution: $\sigma / Q_{BB} = 0.05 \%$
 - Therefore, no background peaks anywhere near the energy of interest
 - Background is flat and well understood
 - Background are measured, with no reliance on background modeling
 - All this leads to an excellent likelihood that an observed signal will be convincing





Searching for neutrinoless double-beta decay of ⁷⁶Ge in HPGe detectors, probing additional physics beyond the standard model, and informing the design of the next-generation LEGEND experiment

Source & Detector: Array of p-type, point contact detectors 29.7 kg of 87% enriched ⁷⁶Ge crystals Included 6.7 kg of inverted coaxial, point contact detectors in final run Excellent Energy resolution: 2.5 keV FWHM @ 2039 keV

and Analysis Threshold: 1 keV

Office of

Science

ENERGY

Low Background: 2 modules within a compact graded shield and active muon veto using ultra-clean materials

Reached an ultimate exposure of ~65 kg-yr before removal of enriched detectors for the LEGEND-200 experiment at LNGS Continuing to operate at the Sanford Underground Research Facility with natural detectors for background studies and other physics







2022





Energy Reconstruction and ICPC Detectors



Energy estimated via optimized trapezoidal filter of ADC-nonlinearity-corrected* traces with charge-trapping correction

FWHM of 2.5 keV at $Q_{\beta\beta}$ of 2039 keV (0.12%) is a record for $0\nu\beta\beta$ searches



FWHM of combined enriched detectors in the MAJORANA DEMONSTRATOR, measured using ²²⁸Th calibration data

NIMA 872 (2017) 16 * IEEE Trans. on Nuc Sci 10.1109/TNS.2020.3043671



MAJORANA operated 4 Inverted-Coaxial Point Contact Detectors from Aug. 2020 to Mar. 2021

- Larger range of drift times requires new analysis techniques
- Best energy resolution for ICPCs to date!



Combined energy resolution of ICPCs improved from 2.9 keV to 2.4 keV FWHM at 2039 keV with new technique

Analysis Techniques for Reducing Backgrounds

0vββ is most likely single-site and located in the bulk of the detector. Many backgrounds are multi-site or located near detector surfaces. Pulse-shape discrimination is used to distinguish between these event topologies.



Operated in a low background regime, benefiting from excellent energy resolution



Full spectrum with combined total of 65 kg-yr.



Results





LEGEND Approach: Proven Technologies



GERDA achieved the lowest background rate: 5x10⁻⁴ cts/(keV kg yr)

LEGEND-200 plans to improve by only x2.5



Combine the best of GERDA:

- LAr active veto and instrumentation
- Low-A shielding, no Pb

MAJORANA achieved best energy resolution: 2.5 keV FWHM at $Q_{\beta\beta}$

LEGEND plans to maintain this performance



... with the best of MAJORANA:

- Radiopurity of near-detector parts
- Low-noise electronics improves PSD

and techniques developed in both experiments:

- Clean fabrication techniques
- Control of surface exposure
- Development of large point-contact detectors

LEGEND Approach: Phased Deployment





arXiv: 2107.11462

LEGEND-200:

- 200 kg, upgrade of existing GERDA infrastructure at Gran Sasso
- 2.5 keV FWHM resolution
- Background goal
 < 0.6 cts/(FWHM t yr)
 < 2x10⁻⁴ cts/(keV kg yr)
- Now in commissioning, physics data starting in 2022

LEGEND-1000:

- 1000 kg, staged via individual payloads (~400 detectors)
- Timeline connected to review process
- Background goal <0.025 cts/(FWHM t yr),<1x10⁻⁵ cts/(keV kg yr)
- Location to be selected



LEGEND-200 Design and Commissioning



Improvements from GERDA/MJD:

- Larger detectors
- Improved LAr light collection: higher purity Ar and improved readout
- Cleaner, lower mass cables
- Lower noise electronics
- UGEFCu and self-vetoing PEN plated for detector mounts

 \rightarrow Factor of 3 reduction in backgrounds relative to GERDA

Quasi-background free operation up to 1 ton-year exposure, for unambiguous discovery up to 10²⁷ yrs



Photo: Enrico Sacchetti



First integrated commissioning run now underway: 4 strings of HPGe detectors, operating with full LAr system D U O

LEGEND-1000 Background Projections



Improvements from LEGEND-200:

- Larger detectors (2.6 kg avg)
- New cables and ASIC read-out
- Underground Ar surrounding detectors
- Optimized array spacing and LAr instrumentation
- Deeper underground site or additional neutron shielding & tagging: SNOLAB and LNGS options

Projected background index after all cuts: $9.4^{+4.9}_{-6.3} \times 10^{-6} \text{ counts/(keV kg yr)}$

> Quasi-background free operation up to 10 ton-year exposure, for unambiguous discovery beyond 10²⁸ years

The LEGEND-1000 Background Model



LEGEND Status

FEGEND

LEGEND-200:

- Upgrade and stand-alone commissioning of the LAr system completed
- 2020 ICPC deployment in LAr with LEGEND electronics demonstrated excellent energy resolution
- First integrated commissioning run now underway!
- First physics data-taking this year

Initial Commissioning: 4 Detector Strings *Ongoing* Follow-up Commissioning & Physics Data: 10 Detector Strings *Fall 2022*

LEGEND-200 Final Goal: 14 Detector Strings *2023*

LEGEND-1000:

- Pre-Conceptual Design Report: arXiv: 2107.11462
- Developing a conceptual design with an refined technical design and background model, proceeding to CD-1
- R&D activities are ongoing





Currently underway: 4 string commissioning

Multi-Site Event Cut

Amplitude of current pulse is suppressed for a multi-site event compared to a single-site event of the same event Energy (AvsE)

- Tuned on ²²⁸Th calibration data to accept 90% of single-site double-escape events. Rejects >50% of the Compton continuum near Qββ
- Corrections applied to AvsE for dependence on energy and drift time have improved signal acceptance by ~6%



Barbeau, Collar, and Tench, J. Cosm. Astro. Phys. 0709 (2007).





Single-site event

Multi-site event

ββ

Surface Cuts: Passivated Surface and Point Contact Events



2022

 α -particles incident on the passivated surface and point contact have a degraded energy reconstruction and can fall near $Q_{\beta\beta}$

- Events far from point contact exhibit slow (~10 µs) charge collection and rising tail slope: cut using Delayed Charge Recovery (DCR), tune to keep 99% of bulk events
- Events near point contact can evade DCR cut, but have fast drift times: cut using high AvsE, tune to keep 98% of bulk events



Joint A/E-DCR spectrum from TUBE scanner, with an α-source scanning across the passivated surface of a PPC detector





EPJC 82 (2022) 226 r, with an α -source f a PPC detector

Gruszko

lulieta

Surface Cuts: Transition Dead-Layer Events

Events in lithiated n-plus surfaces experience energy degradation and slow (~1-2 μs) rerelease of charge. Events with a partial charge deposit in this transition layer are potential backgrounds!

- Cut waveforms with a slow component using "Late Charge" (LQ): area above rising edge of waveform after 80% of charge is collected
- Tune to keep >99% of single-site bulk events using ²⁰⁸Tl double escape events











Inverted Coaxial Point Contact Detectors

Inverted coaxial point contact (ICPC) detectors are larger (1.4 - 2.1 kg) than PPC detectors (0.6 - 1.2 kg). MAJORANA operated 4 ICPCs from Aug. 2020 to Mar 2021

- Beneficial for background reduction in LEGEND
- Larger range of drift times requires more refined analysis techniques
- MAJORANA has demonstrated comparable performance with ICPCs and PPCs. Best energy resolution for ICPCs to date!





New analysis techniques improve combined energy resolution of ICPCs from 2.9 keV to 2.4 keV FWHM at 2039 keV