MJD DATA RELEASE ANALYSIS

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Contents

1. Introduction

Introduction

- **Neutrinoless Double-Beta Decay (NLDBD)**
  - The Majorana Demonstrator experiment searched for neutrinoless double-β decay (0νββ) of 76Ge using modular arrays of 56 high-purity Ge (HPGe) detectors.
- **Dataset:** Four files provided: Detector A, Detector B, Detector C, Detector Target.
  - Each record contains:
    - Event ID – unique identifier
    - Classification Score (0–1) – produced by a neural network
    - Energy (keV) – measured energy of each event
- **Project Objective:** To simulate a realistic 0νββ search workflow by:
  - Extract detector energy spectra
  - Assess signal–background discrimination performance
  - Fit the unknown contribution of Detector C and the possible NLDBD signal using a statistical model.

2. Methodology

Overview

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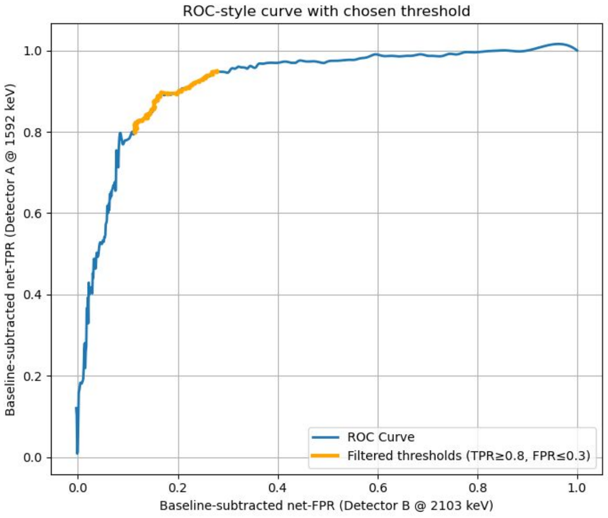
- **Data preparation & Efficiency Extraction:**
  - **Input Generation:** Detector Datasets → Normalized Energy PDFs
  - **Metric Extraction:**
    - Detector A: Net-TPR
    - Detector B: Net-FPR
- **Threshold Optimization: TPR ≥ 0.8 and FPR ≤ 0.3**
  - a classifier-driven method that maximizes Youden's J = TPR − FPR,
  - ✓ a **physics-driven method** that evaluates all allowed thresholds to find the one that produces the best sensitivity.
- **Likelihood Fit & Results**
  - **Model Construction:** Build Post-cut PDFs (Detectors A, B, C & Target)
    - Frequentist Poisson-Likelihood Fit ($\mu = \theta_A P_A + \theta_B P_B + \theta_C P_C + \theta_N P_N$)
  - **Final Output**: 90% CL Upper Limit on θ_N; Experimental Sensitivity



Step 1: Energy Spectrum Construction

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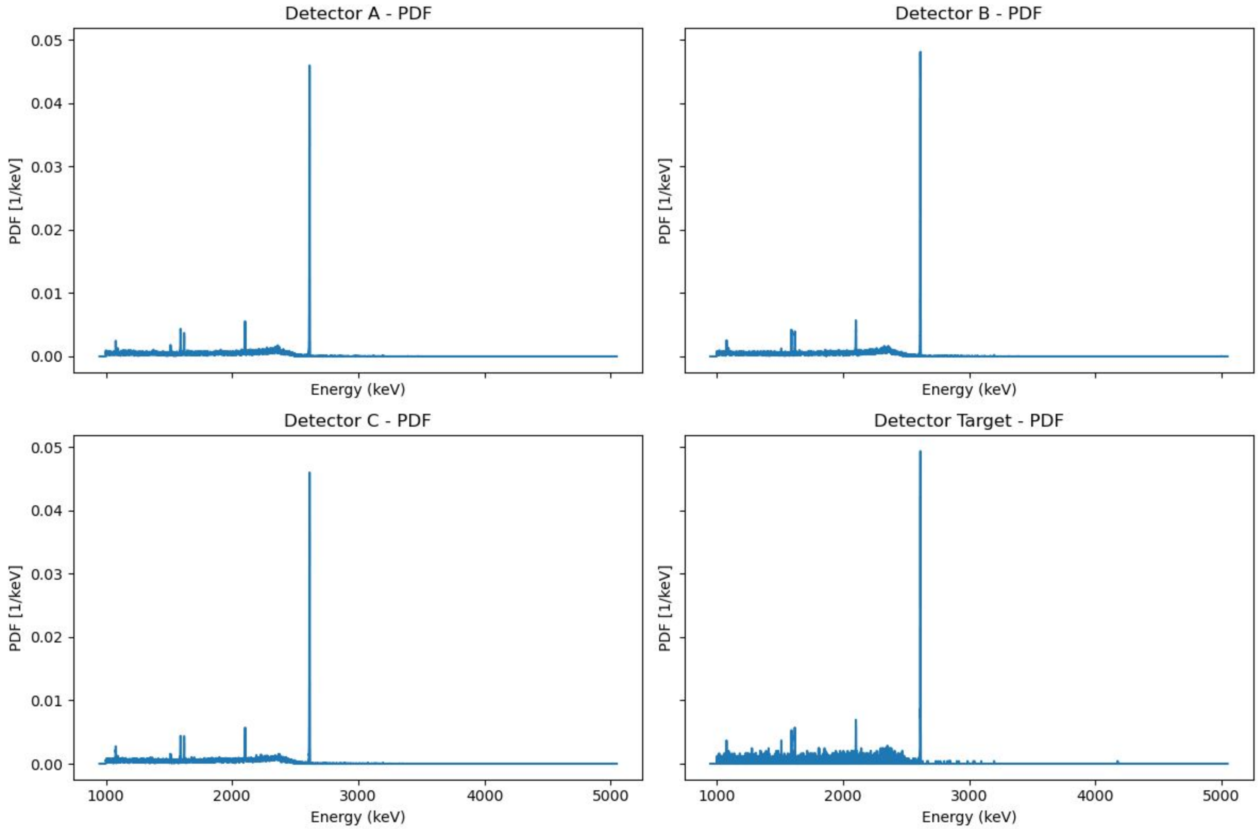
- Goal: Convert raw event-level CSV data into energy spectra for Detectors A, B, C, and Target.
- Defining the Histogram Bin Content
- Produce both:
  - Histogram counts (events per bin)
  - Normalized PDFs (probability density functions)

```
=== Detector A ===
shape: (40000, 3)
score range: [0.0000, 0.9720]   energy range: [1000.02, 3475.61] keV

=== Detector B ===
shape: (40000, 3)
score range: [0.0000, 0.9630]   energy range: [1000.01, 4998.51] keV

=== Detector C ===
shape: (40000, 3)
score range: [0.0000, 0.9710]   energy range: [1000.11, 3351.51] keV

=== Detector Target ===
shape: (4902, 3)
score range: [0.0000, 0.9630]   energy range: [1000.01, 4177.60] keV

Global data energy range: [1000.01, 4998.51] keV
Analysis binning: E_MIN=950.0 keV, E_MAX=5048.5 keV, BINW=0.50 keV
Number of bins = 8197
```

Step 1: Energy Spectrum Construction

- Normalized PDF:



Step 2

Goal: Estimate how many true signal events survive a Classification Score threshold, using the 1592 keV signal peak in Detector A.

1. Define Peak & Sideband Energy Windows
   - **Signal peak window:** [1592 – 3, 1592 + 3] keV
     (contains signal + small background)
     Sideband windows: [1592 − 9,1592 − 3] keV + [1592 + 3,1592 + 9] keV
     (represent background only)
   - Extract the **Classification Score** for each event from these regions
   - Calculate the **background scaling factor**:

$$\alpha = \frac{\textit{peak width}}{\textit{sideband width}} = \frac{6}{12} = 0.5$$

This factor determines the number of background that would normally be in the peak.

2. Construct Threshold Grid Using Peak-Score Quantiles
   - **Generate 250 candidate thresholds** by taking quantiles of the **peak-window score distribution**
     Reason for using quantiles instead of fixed steps (0–1):
     Peak-score distribution is not uniform. Quantiles ensure sampling is dense where signal scores cluster, and do not waste grid points in empty score regions.
   - Remove duplicates (If many peak scores repeat, multiple quantiles may map to the same value.)

3. Compute Net-TPR for Each Threshold

- **Baseline-subtracted True Positive Rate**

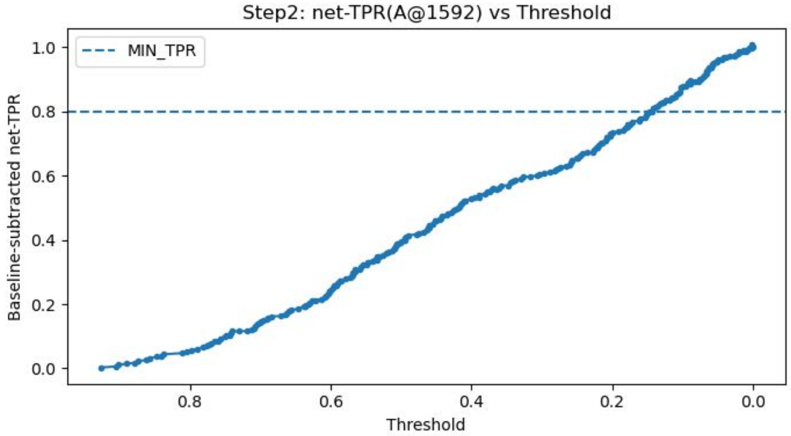
  (Net passed signal events / Net total signal in peak)

$$\mathrm{TPR}_{net}(t) = \frac{N_{pass,peak}(t) - \alpha N_{pass,sb}(t)}{N_{peak} - \alpha N_{sb}}$$

This yields the fraction of true signal events retained after applying threshold t, with background contamination removed.

Reason for using baseline-subtracted TPR:

The 1592 keV peak contains both signal and residual background, and background subtraction (using sidebands) is required to obtain an unbiased estimate of the true signal retention efficiency.



4. Results

- Very low thresholds retain nearly all signal
  - Threshold = 0.0000 → TPR ≈ 1.000
  - Threshold = 0.0020 → TPR ≈ 0.9976
- As threshold increases, net-TPR decreases smoothly
  - Threshold ≈ 0.88 → TPR ≈ 0.017
  - Threshold ≈ 0.90 → TPR ≈ 0.011
  - Threshold ≈ 0.93 → TPR < 0.003

Higher score thresholds filter out more background but also remove true signal, causing TPR to fall from 1 to 0.

Step 3

Goal: Evaluate Background Using Detector B @ 2103 keV

1. Define Peak & Sideband Energy Windows (Detector B)
   - **Signal peak window:** [2103 – 3, 2103 + 3] keV
     Sideband windows: [2103 − 9,2103 − 3] keV + [2103 + 3,2103 + 9] keV
   - Extract the **Classification Score** for each event from these regions
   - Calculate the **background scaling factor**: $\alpha_B = \frac{\textit{peak width}}{\textit{sideband width}} = \frac{6}{12} = 0.5$

2. Apply thresholds from Step 2
3. Compute Net-FPR
   - **Baseline-subtracted net FPR :** $\text{net } FPR = \frac{N_{pass,peak} - \alpha N_{pass,sb}}{N_{peak} - \alpha N_{sb}}$
   - Iterate over thresholds from Step 2:
   - **Peak region:** count how many events have scores ≥ threshold ⟶ potential false positives
   - **Sideband regions:** count how many events have scores ≥ threshold ⟶ the background contribution, which is subtracted from the peak count.
   - Compute Net-FPR

This estimate background leakage under the same thresholds used for signal.

4. Merge Signal & Background Rates

- **net-TPR (A@1592) vs Threshold:**

  At higher thresholds → net signal efficiency gradually decreases

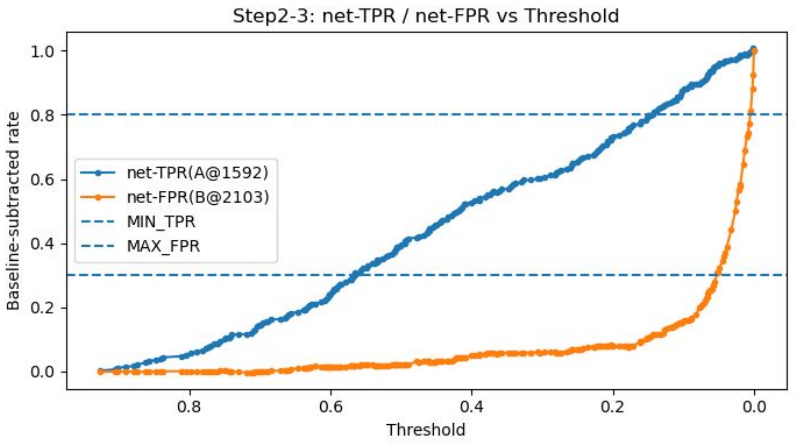
  Thresholds that maintain high TPR (> MIN_TPR) cover a reasonably wide range

- **net-FPR (B@2103) vs Threshold:**

  Lower thresholds → high background false positives (1.0)

  Increasing threshold → FPR rapidly decreases

  Slight negative net-FPR values (-0.001) occur due to baseline subtraction, which is normal



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5. Filter Acceptable Thresholds

- **Filtering criteria:**

$$\mathrm{TPR\_A1592\_net} \geq \mathrm{MIN\_TPR} \quad \& \quad \mathrm{FPR\_B2103\_net} \leq \mathrm{MAX\_FPR}$$

- **Results from Filtering:**
  - Total thresholds scanned: 246
  - Thresholds satisfying both criteria: 38
  - Higher thresholds → lower net-FPR but slightly reduced net-TPR
    Lower thresholds → higher net-TPR but risk exceeding MAX_FPR

Final candidate thresholds balance **high signal TPR** and **low background FPR**.

- Example of remaining candidates:

thr	TPR_A1592_net	FPR_B2103_net
0.056	0.949	0.278
0.059	0.937	0.258
0.065	0.925	0.242
0.070	0.906	0.215

Step 4

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Goal:

- Represent the 0νββ (NLDBD) signal at 2039 keV as a Gaussian.
- Construct a binned probability density function (PDF) for use in analysis or likelihood fits.

Methods:

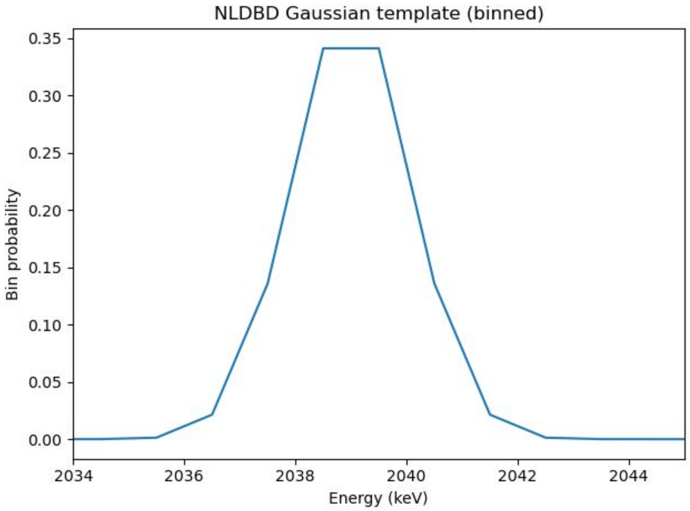
1. Define energy bins: 500–3000 keV, **1 keV width**.
2. Compute Gaussian probability for each bin:

$$p_i = P(E \in [edge_i, edge_{i+1}]) = CDF(edge_{i+1}) - CDF(edge_i)$$

- Normalize, then $\sum_i p_i = 1$.

3. Gaussian parameters:

- Mean: 2039 keV
- Sigma: 1 keV



Result:

- PDF is sharply peaked around 2039 keV.
- Most probability concentrated in **2038–2040 keV**, forming a smooth discrete Gaussian shape.
- Outside this range, bin probabilities quickly drop to near zero.

Step 5

Goal:

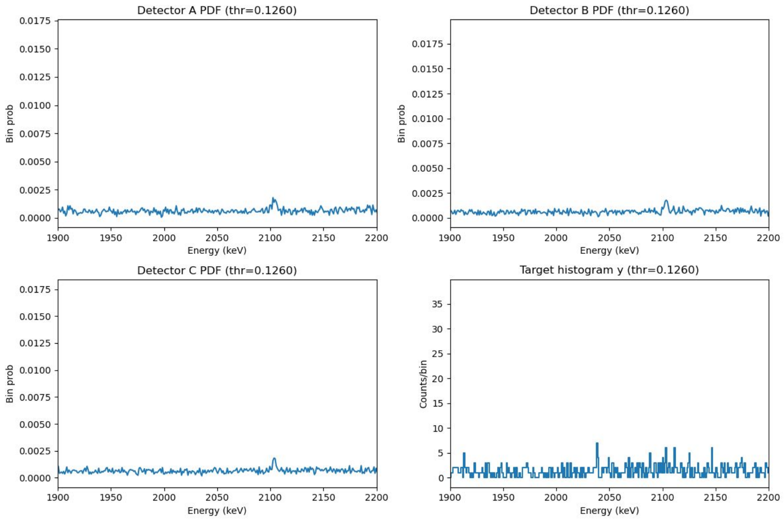
- Apply a classification score cut to all detectors.
- Generate:
  - Normalized PDFs for detectors A, B, C
  - Histogram counts for DetectorTarget

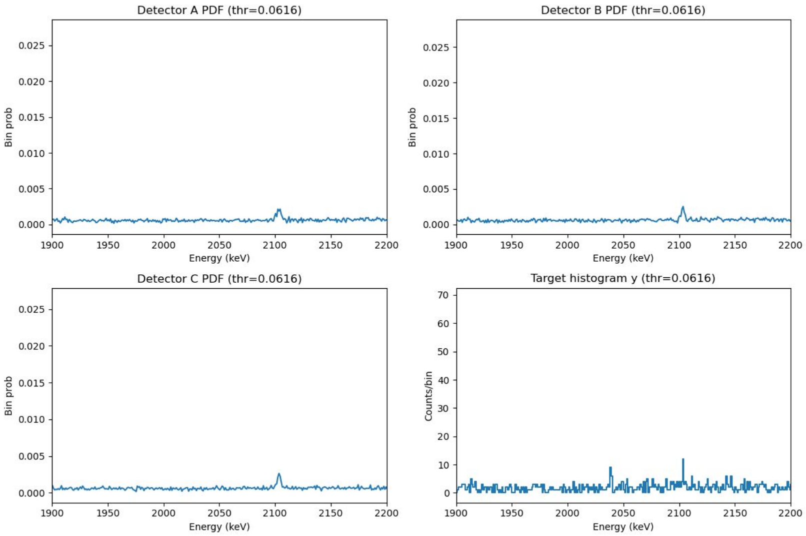
Methods:

1. Apply Cut
   - Filter events in all detectors (A, B, C, Target) based on a classification score threshold.
   - Keep only events with high confidence to reduce background or low-score events.
2. Build Target Histogram
   - For the filtered Target detector, create a histogram of energy values.
   - The histogram represents absolute counts per energy bin.
3. Build PDFs for Detectors A, B, C
   - For each filtered detector (A, B, C), create normalized probability distributions (PDFs).
   - Each PDF shows the shape of the energy distribution after applying the cut.

Threshold (thr)	A2 events	B2 events	C2 events	Target events	Target counts sum
0.0616	22,801	22,836	22,724	2,793	2,793
0.0778	20,729	20,804	20,786	2,562	2,562
0.0980	18,786	18,891	18,853	2,311	2,311
0.1260	16,666	16,810	16,889	2,059	2,059

- As the threshold increases:
  - Number of events in all detectors decreases.
  - Target histogram counts gradually decrease.
- Provides a clear picture for selecting an optimal threshold.





Step 6：Frequentist fit

- **Goal:** Fit the entire Target energy spectrum after applying a CNN score threshold, and estimate the event yields
- **input:**（after applying the CNN score cut）
  target histogram count(unnormalized) y; P_A P_B P_C P_{NLDBD} PDF(normalized)
- **constraints:** θ >= 0
- **calibration information:** $\theta_A = 1350 \pm 100$ & $\theta_B = 770 \pm 270$
- **optimization:**

  (1) $\mu = \theta_A P_A + \theta_B P_B + \theta_C P_C + \theta_N P_N$

  (2) NLL = $\Sigma(\mu - y\log\mu)$ + penalty(A) + penalty(B), penalty(A) = $[(\theta_A - 1350)/100]$ ^ 2 / 2, penalty(B) = $[(\theta_B - 770)/270]$ ^ 2 / 2
- **output:** best fit θ_A θ_B θ_C θ_N per threshold & NLL_{min}

Step 6 : Frequentist fit

- **Obtain the θ's : Numerical optimization**

  (1) Choose an initial guess x0 (typically starting from the calibration means).

  (2) Use L-BFGS-B, which supports bound constraints ($\theta \geq 0$).

  (3) Iteratively update θ to reduce the total objective NLL_total (Poisson NLL + Gaussian penalties).

  (4) When the optimizer converges, it returns the best-fit parameters in res.x

  (5) Finally:

  thetaA_hat, thetaB_hat, thetaC_hat, thetaN_hat = res.x

Step 6 : Frequentist fit

	thr	fit_success	nll_min	thetaA_hat	thetaB_hat	thetaC_hat	thetaN_hat	Target_counts_sum
0	0.0560	True	437.5416	1213.7459	878.1503	806.2143	12.1475	2898.0
1	0.0570	True	474.1626	1218.4828	901.1685	749.6507	12.1769	2870.0
2	0.0580	True	500.9856	1212.0838	869.7536	773.5249	12.1682	2855.0
3	0.0597	True	534.6665	1204.1188	865.2729	756.8711	12.1775	2825.0
4	0.0616	True	561.4315	1188.3163	872.4645	734.9684	12.2340	2793.0
5	0.0620	True	561.4315	1188.3163	872.4645	734.9684	12.2340	2793.0
6	0.0640	True	577.3998	1180.6151	891.4499	689.1737	12.2522	2757.0
7	0.0650	True	583.6953	1176.8650	886.3042	683.5515	12.2473	2742.0
8	0.0660	True	596.9032	1179.2527	881.1225	671.1255	12.2587	2727.0
9	0.0676	True	612.0850	1177.3898	878.1871	660.2492	12.2612	2711.0
10	0.0694	True	632.5966	1177.3962	881.2156	632.9353	11.3862	2686.0
11	0.0709	True	643.0279	1174.6121	877.8137	622.4375	11.3886	2669.0
12	0.0736	True	698.1229	1173.8737	895.9754	560.8264	11.4753	2625.0
13	0.0760	True	736.0257	1168.4426	890.5702	540.1386	11.6077	2593.0
14	0.0778	True	757.1926	1166.2829	839.6753	563.0448	11.5990	2562.0
15	0.0817	True	840.8847	1159.2380	825.6731	526.9052	10.6619	2504.0
16	0.0880	True	907.9516	1142.1390	785.5603	509.9899	10.8974	2428.0
17	0.0891	True	933.2212	1138.3090	758.6673	518.3348	10.8910	2405.0
18	0.0920	True	955.6276	1137.7890	741.8359	513.0929	8.7054	2380.0
19	0.0952	True	968.6855	1135.6317	727.0206	490.1627	8.9416	2339.0
20	0.0980	True	985.4946	1130.6443	710.4807	484.2139	9.0205	2311.0
21	0.1014	True	1018.1018	1123.4730	670.3671	488.6186	8.8649	2267.0
22	0.1020	True	1018.1018	1123.4730	670.3671	488.6186	8.8649	2267.0
23	0.1044	True	1031.5594	1111.7705	661.8057	489.9445	8.9627	2247.0
24	0.1058	True	1036.0320	1110.7050	663.1473	481.6972	8.9509	2239.0
25	0.1080	True	1024.9556	1108.4129	655.7178	470.5519	9.1263	2217.0
26	0.1110	True	1042.5005	1114.2484	640.0806	447.8888	9.2433	2185.0
27	0.1132	True	1053.8181	1108.5939	633.7202	438.3948	9.2460	2163.0
28	0.1160	True	1062.0570	1102.2135	622.9935	435.1010	9.2475	2142.0
29	0.1190	True	1074.0849	1100.7293	623.3139	410.3613	9.2549	2116.0
30	0.1230	True	1097.8162	1095.0847	583.0638	423.9390	9.2778	2083.0
31	0.1260	True	1115.7523	1070.3626	578.5116	431.2760	9.3168	2059.0
32	0.1290	True	1131.5756	1056.3518	589.3244	412.4334	9.3335	2036.0
33	0.1317	True	1139.2324	1034.7833	565.4335	434.5916	9.3755	2011.0
34	0.1358	True	1177.0976	1024.6424	553.8743	424.6611	8.7470	1978.0
35	0.1379	True	1187.9795	1018.6398	549.1984	420.7960	8.8278	1963.0
36	0.1410	True	1204.1397	1019.1015	551.2740	401.1565	8.8622	1946.0
37	0.1433	True	1221.3495	1008.8132	518.8914	422.6959	7.8246	1923.0

Figure 1. Results for Step 6 after fitting

Step 7: 90% confidence upper limit on θ_N

- **Goal:** Compute the observed one-sided 90% confidence level upper limit on θN using a Frequentist profile likelihood
- **input:**（input + output of step 6）
  target histogram count(unnormalized) y; P_A P_B P_C P_{NLDBD} PDF(normalized)
  best fitness: thetaA_hat, thetaB_hat, thetaC_hat, thetaN_hat
- **constraints:** θ >= 0
- **calibration information:** $\theta_A = 1350 \pm 100$ & $\theta_B = 770 \pm 270$
- **profile likelihood:**

  (1) $NLL_{prof}(t) = \min\{NLL(\theta_A, \theta_B, \theta_C, \theta_N = t)\}$

  (2) $q(t) = 2 *(NLL_{prof}(t) - NLL_{min})$, $q(t) = 2.71$ according to Wilks approximation
- **output:** $UL_{90} = \min\{t >= thetaN\_hat \mid q(t) = 2.71\}$

Step 7: 90% confidence upper limit on θ_N

(1) Start from $t_0=\max(\theta_N,0)$

(2) Increase t until q(t) >= 2.71(bracketing)

(3) Solve q(t) = 2.71 numerically

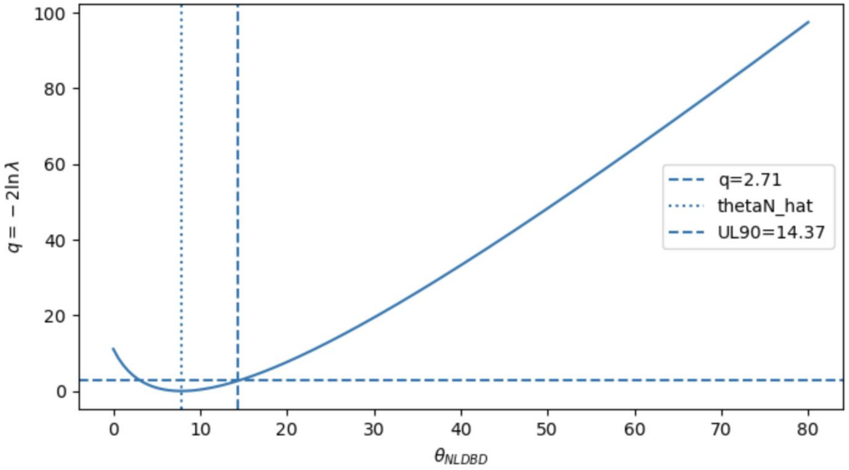


Figure 2. One Sample q(t) – θN results

Step 7: 90% confidence upper limit on θ_N

	thr	TPR_A1592_net	FPR_B2103_net	fit_success	thetaN_hat	UL90	nll_min
0	0.0560	0.9490	0.2780	True	12.1475	20.0511	437.5416
1	0.0570	0.9465	0.2686	True	12.1769	20.0819	474.1626
2	0.0580	0.9417	0.2686	True	12.1682	20.0730	500.9856
3	0.0597	0.9368	0.2575	True	12.1775	20.0804	534.6665
4	0.0616	0.9344	0.2541	True	12.2340	20.1391	561.4315
5	0.0620	0.9344	0.2541	True	12.2340	20.1391	561.4315
6	0.0640	0.9283	0.2489	True	12.2522	20.1636	577.3998
7	0.0650	0.9247	0.2421	True	12.2473	20.1611	583.6953
8	0.0660	0.9198	0.2327	True	12.2587	20.1748	596.9032
9	0.0676	0.9149	0.2275	True	12.2612	20.1839	612.0850
10	0.0694	0.9101	0.2216	True	11.3862	19.0987	632.5966
11	0.0709	0.9064	0.2147	True	11.3886	19.1018	643.0279
12	0.0736	0.9016	0.2062	True	11.4753	19.1853	698.1229
13	0.0760	0.9004	0.2027	True	11.6077	19.3176	736.0257
14	0.0778	0.8943	0.1976	True	11.5990	19.3112	757.1926
15	0.0817	0.8943	0.1788	True	10.6619	18.1565	840.8847
16	0.0880	0.8967	0.1668	True	10.8974	18.4003	907.9516
17	0.0891	0.8870	0.1642	True	10.8910	18.3935	933.2212
18	0.0920	0.8882	0.1600	True	8.7054	15.7534	955.6276
19	0.0952	0.8797	0.1583	True	8.9416	15.9948	968.6855
20	0.0980	0.8797	0.1574	True	9.0205	16.0860	985.4946
21	0.1014	0.8748	0.1523	True	8.8649	15.8571	1018.1018
22	0.1020	0.8748	0.1523	True	8.8649	15.8571	1018.1018
23	0.1044	0.8615	0.1523	True	8.9627	15.9590	1031.5594
24	0.1058	0.8566	0.1514	True	8.9509	15.9519	1036.0320
25	0.1080	0.8542	0.1471	True	9.1263	16.1193	1024.9556
26	0.1110	0.8457	0.1446	True	9.2433	16.2366	1042.5005
27	0.1132	0.8433	0.1411	True	9.2460	16.2428	1053.8181
28	0.1160	0.8408	0.1369	True	9.2475	16.2447	1062.0570
29	0.1190	0.8360	0.1386	True	9.2549	16.2561	1074.0849
30	0.1230	0.8348	0.1343	True	9.2778	16.2804	1097.8162
31	0.1260	0.8287	0.1283	True	9.3168	16.3314	1115.7523
32	0.1290	0.8262	0.1198	True	9.3335	16.3434	1131.5756
33	0.1317	0.8226	0.1155	True	9.3755	16.3901	1139.2324
34	0.1358	0.8177	0.1138	True	8.7470	15.5360	1177.0976
35	0.1379	0.8129	0.1146	True	8.8278	15.6162	1187.9795
36	0.1410	0.8080	0.1163	True	8.8622	15.6533	1204.1397
37	0.1433	0.8007	0.1138	True	7.8246	14.3726	1221.3495

Figure 3. Results of Step 7 for 90% confidence UL

Step 8 Sensitivity (Median Expected 90% Upper Limit)

❖ What is Sensitivity

The median 90% Bayesian/Frequentist upper limit obtained by repeating many hypothetical experiments under the no-signal assumption。

❖ Workflow of Sensitivity Calculation

Step 1 — **Step 2** — **Step 3** — **Step 4**

- Step 1: Determine Truth Model
- Step 2: Generate Toy Experiments
- Step 3: For Each Toy, Compute Its 90% Upper Limit
- Step 4: The median of the distribution of UL90 values

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Step 8

Determine Truth Model

1. Fix the signal strength to zero
2. Perform a profile likelihood fit to the real data.
3. Extract the best-fit background normalizations: $\theta_A^0,\ \theta_B^0,\ \theta_C^0.$
4. Construct the "true" expectation spectrum:

$$\mu_{\text{true}}(E) = \theta_A^0 p_A(E) + \theta_B^0 p_B(E) + \theta_C^0 p_C(E)$$

Step 8

Generate Toy Experiments

1. For each energy bin, generate toy data: $y_{\text{toy}}(E) \sim \text{Poisson}(\mu_{\text{true}}(E))$
2. Each toy represents a possible experimental outcome when no NLDBD signal exists.
3. Quick scan: start with N_toys=30 to test the procedure and scan thresholds.
4. Final evaluation: increase to N_toys=100~200 for a more precise estimate of the median 90% upper limit.

Step 8

For Each Toy, Compute Its 90% Upper Limit :

1. Perform a full fit on the toy data → obtain θA,θB,θC,θN and the minimum NLL.

2. Scan over fixed θN and compute:

$$q(\theta_N) = 2\left[\mathrm{NLL}_{\mathrm{profile}}(\theta_N) - \mathrm{NLL}_{\mathrm{min}}\right]$$

3. Find the value where:

$$q(\theta_N) = 2.71$$

→ this defines the 90% upper limit for that toy.

Step 8

Optimizing Sensitivity Across Thresholds :

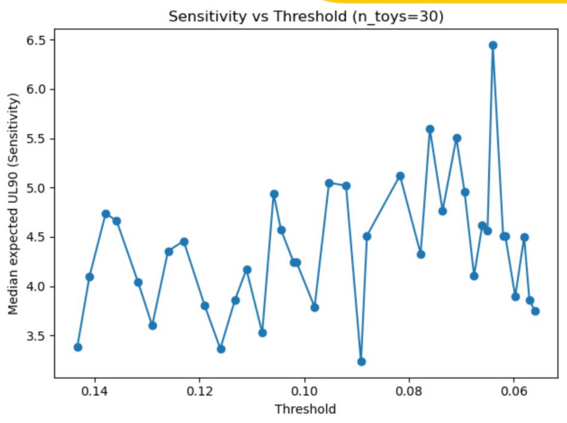
We systematically scan a range of analysis thresholds to evaluate the median expected 90% upper limit (sensitivity) under the no-signal hypothesis. Each row corresponds to a specific threshold value, with its associated True Positive Rate (TPR), False Positive Rate (FPR), and median UL90.

	thr	TPR_A1592_net	FPR_B2103_net	Sensitivity_median_UL
0	0.0560	0.9490	0.2780	3.7485
1	0.0570	0.9465	0.2686	3.8631
2	0.0580	0.9417	0.2686	4.4975
16	0.0880	0.8967	0.1668	4.5118
17	0.0891	0.8870	0.1642	3.2355
18	0.0920	0.8882	0.1600	5.0175
19	0.0952	0.8797	0.1583	5.0486
20	0.0980	0.8797	0.1574	3.7873
21	0.1014	0.8748	0.1523	4.2400
22	0.1020	0.8748	0.1523	4.2400
23	0.1044	0.8615	0.1523	4.5765
24	0.1058	0.8566	0.1514	4.9376
25	0.1080	0.8542	0.1471	3.5274

Step 8

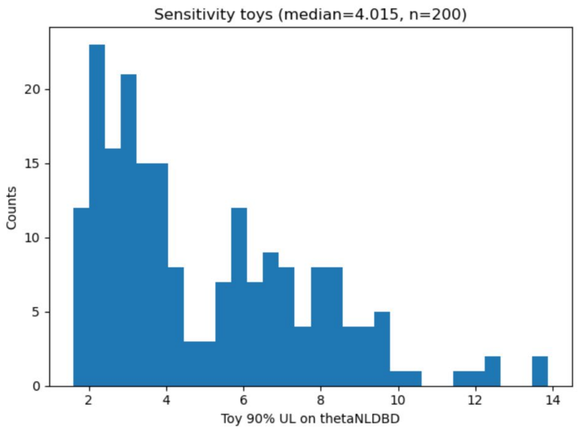
Quick Scan for Optimal Threshold

- Performed a preliminary scan using **30 toy datasets** per threshold.
- Identified the threshold that minimizes the median expected UL:
  Best threshold (quick scan) = 0.0891



Final Sensitivity Evaluation

- Using the selected threshold, we generated **200 toy datasets** to obtain a more precise estimate.
- Resulting **median expected 90% UL (sensitivity) = 4.015**



3. Conclusion

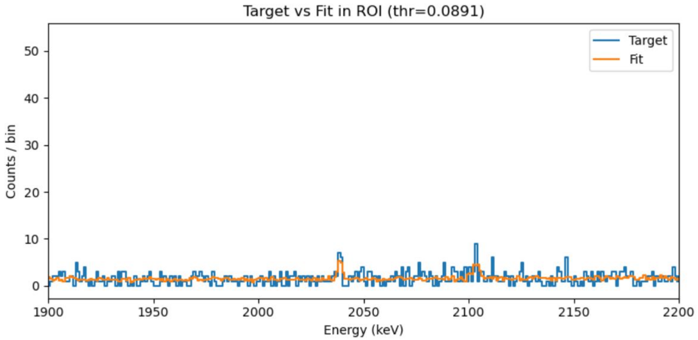
Best Threshold & Fit Results

UC San Diego

1. Best Threshold

- `best_thr = 0.0891`
- Threshold selected to maximize sensitivity while keeping TPR and FPR within acceptable ranges.

2. Fit Results (Step6)

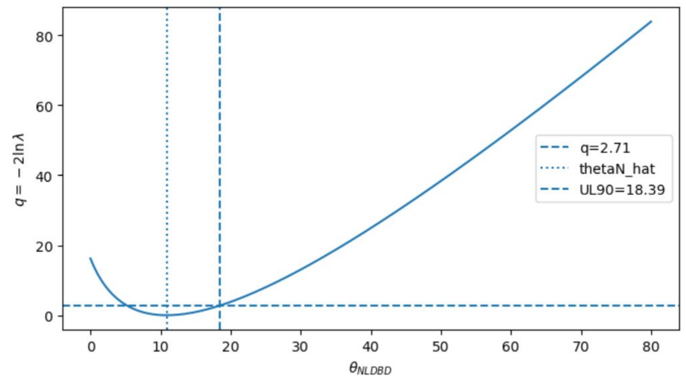


- `θ_A_hat = 1138.31 (calib: 1350 ± 100)`
- `θ_B_hat = 758.67 (calib: 770 ± 270)`
- `θ_C_hat = 518.33`
- `θ_N_hat = 10.89`
- `NLL_min = 933.22`
- `Target total counts after cut = 2405`
- Fit is successful; estimated parameters are consistent with calibration values.

Observed Upper Limit & Sensitivity

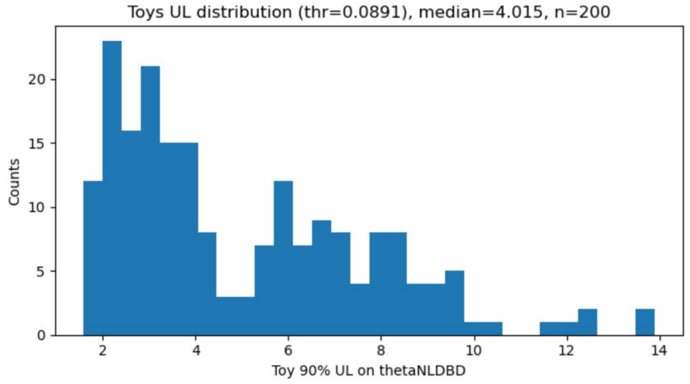
1. Observed Upper Limit (Step7)

- 90% UL on θ_NLDBD = 18.39
- This represents the main physical quantity constrained by the observed data.



2. Sensitivity (Step8)

- Median expected UL = 4.015 (200 toys)
- Sensitivity evaluated via toy experiments confirms the expected performance of the method.



Thank you!