INTERPETABLE MACHINE LEARNING APPROACH FOR ELECTRON ANTINEUTRINO SELECTION

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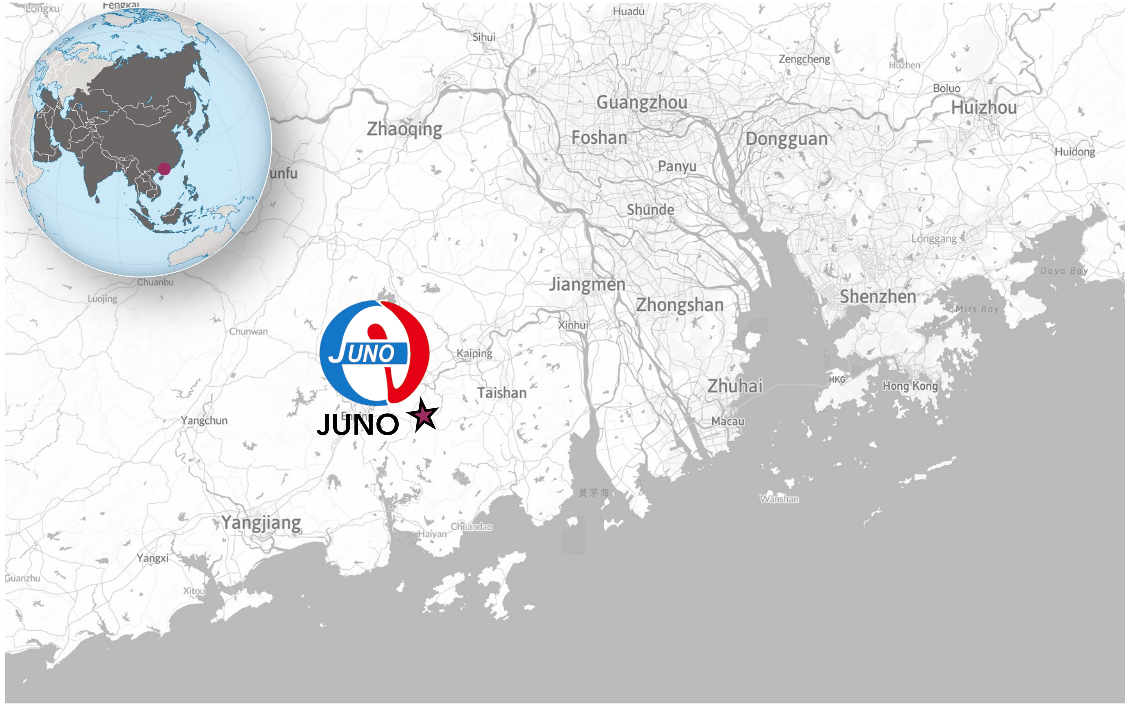
INFN Istituto Nazionale di Fisica Nucleare

Università degli Studi di Padova

JUNO AT A GLANCE

PPNP 123 (2022): 103927

The **J**iangmen **U**nderground **N**eutrino **O**bservatory (**JUNO**) is a multi-purpose neutrino experiment currently under construction in South China.



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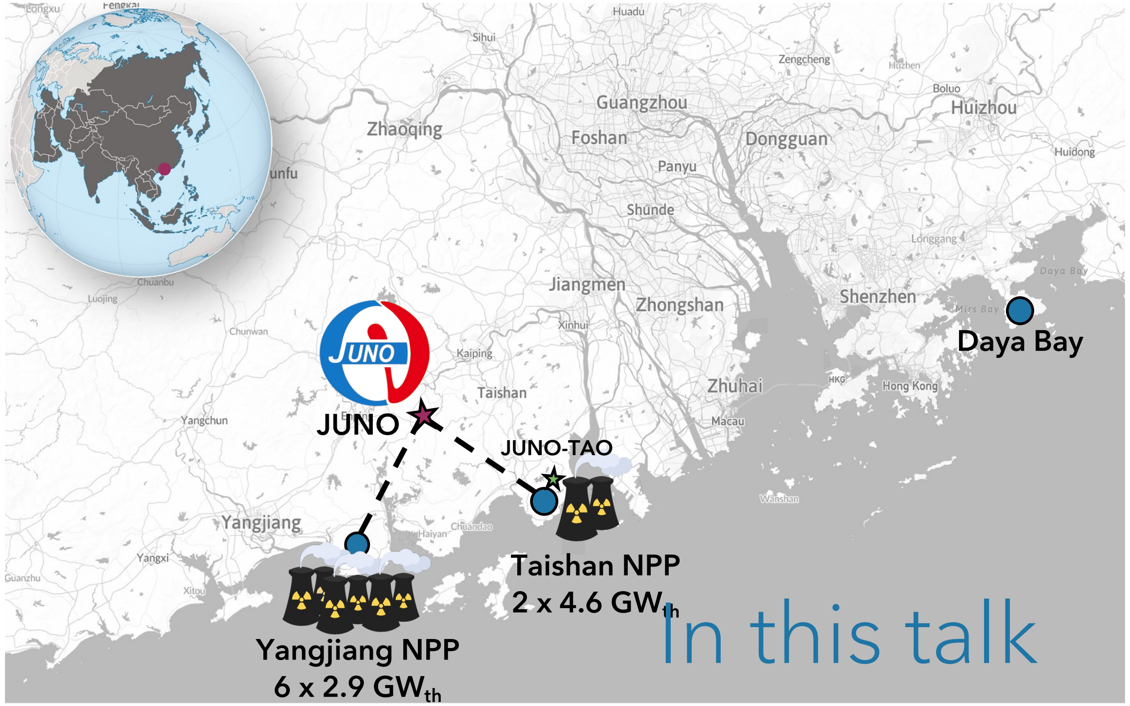
- ✶ 52.5 km from two major Nuclear Power Plants (NPPs) with eight nuclear reactors (26.6 GW_{th})
- ✶ 35 m-diameter sphere with **20 ktons of liquid scintillator** (LS) surrounded by a water Cherenkov detector
- ✶ Unprecedented energy resolution for a LS-based detector → **3% at 1 MeV** arXiv 2405.17860



In this talk

Experiment	Daya Bay	RENO	Double Chooz	KamLAND	JUNO
LS mass	20 ton	16 ton	8 ton	1 kton	20 kton
Energy resolution	8%	8%	8%	6%	3%

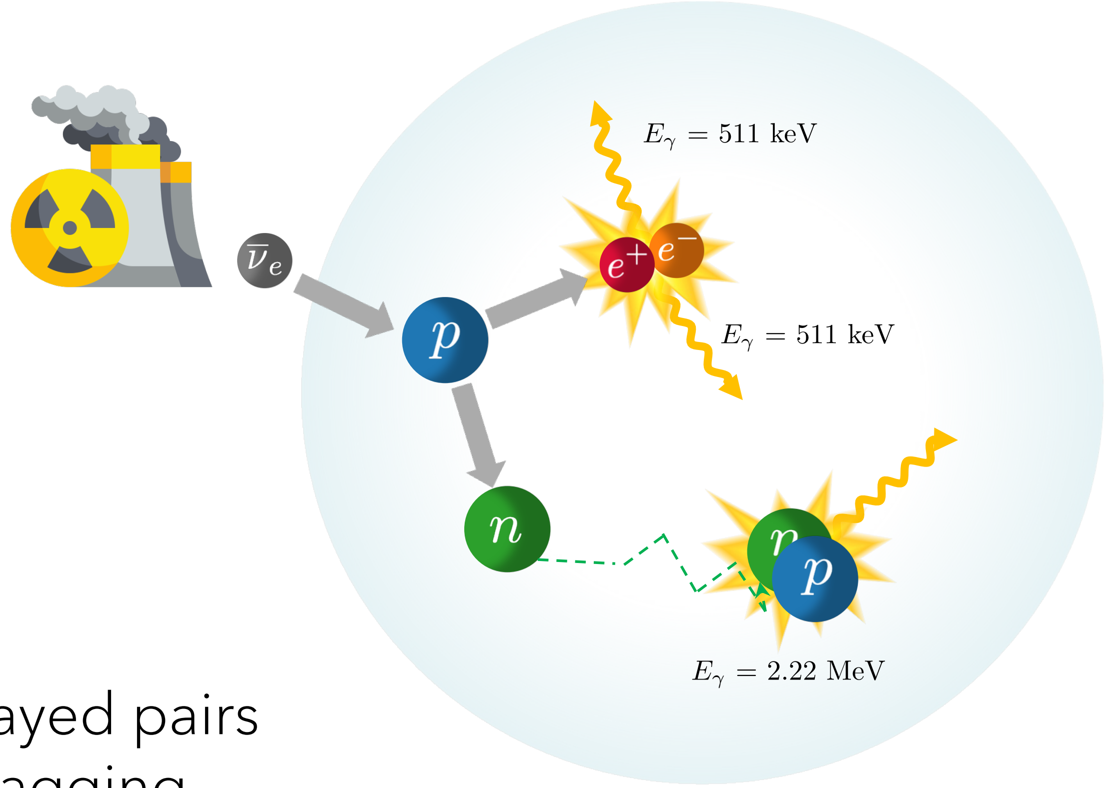
ANTINEUTRINO DETECTION

✶ Primary detection channel is the Inverse Beta Decay (IBD) reaction:

$$\overline{\nu}_e + p \rightarrow e^+ + n$$

Prompt signal: energy deposited by positron + annihilation energy

Delayed signal: neutron capture on nucleus (e.g., Hydrogen, Lithium, Gadolinium) and subsequent gamma ray emission



✶ Close time and space correlation of prompt-delayed pairs
→ efficient background suppression and event tagging

✶ Positron retains most of incoming antineutrino energy

EXPECTED BACKGROUNDS

Backgrounds can be divided into two categories:

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    - Geoneutrinos are electron antineutrinos and interact via IBD → irreducible

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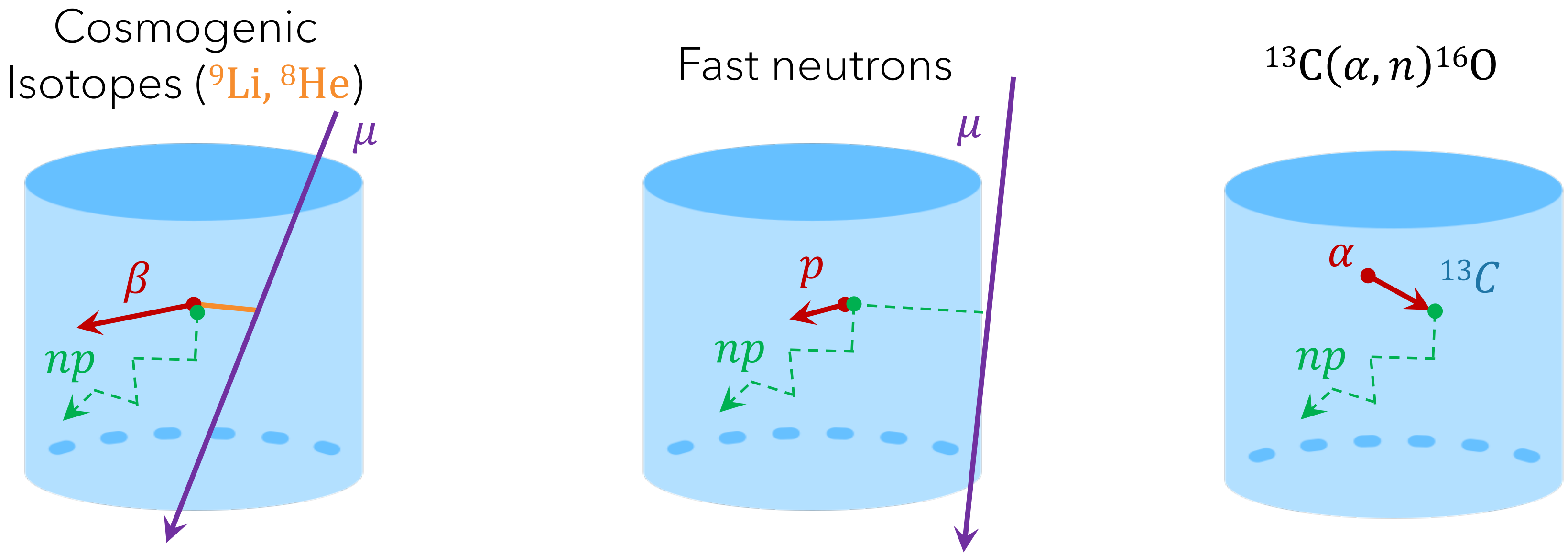

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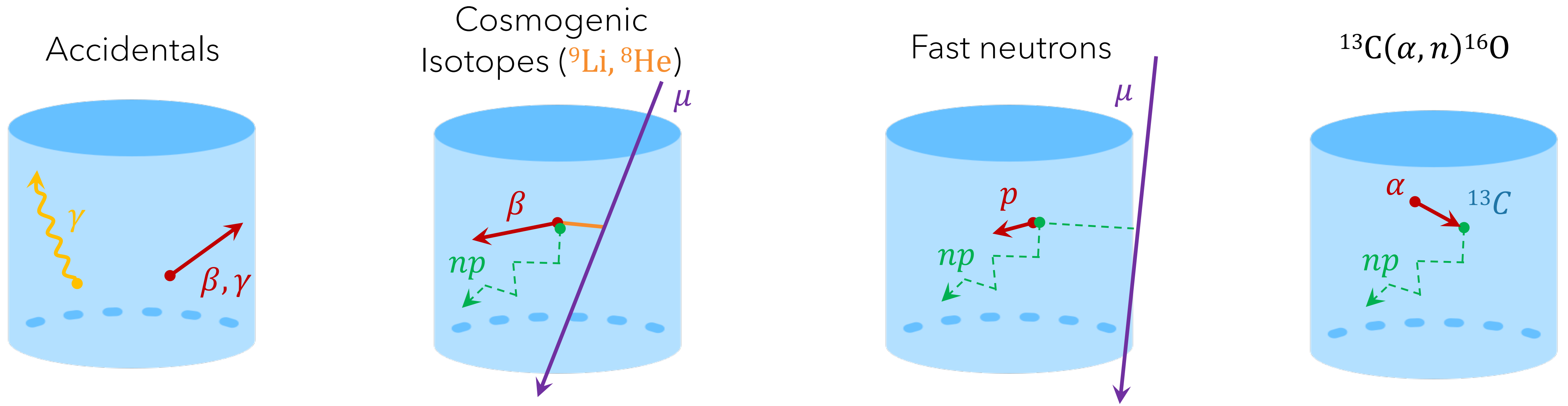
2. **Uncorrelated background:** accidental coincidences
   - Two independent signals (mainly from radioactive contamination) mimic the IBD pattern



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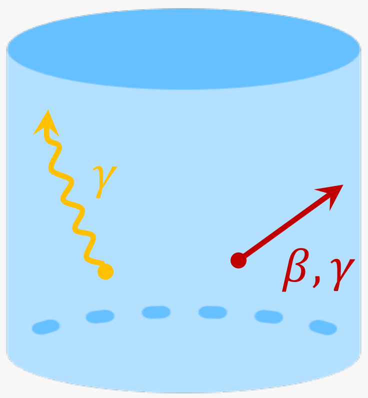
Accidentals



Before any selection, rate of single radioactive events is much higher than expected signal rate

The main task of **a selection algorithm** is **to distinguish between two classes**: reactor antineutrino events and accidental coincidences

DATA DESCRIPTION AND BENCHMARK SELECTION

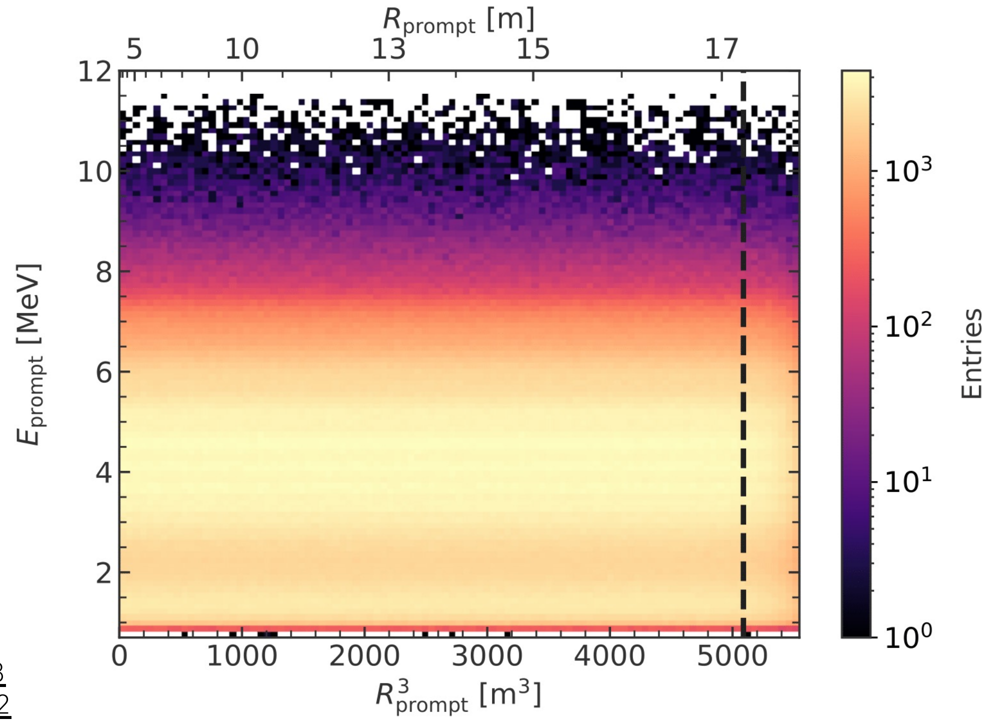
DATA DESCRIPTION

- Highly imbalanced data: 57.4 **IBDs** /day [1] vs >10^5 **accidentals** /day [2] (pairs)

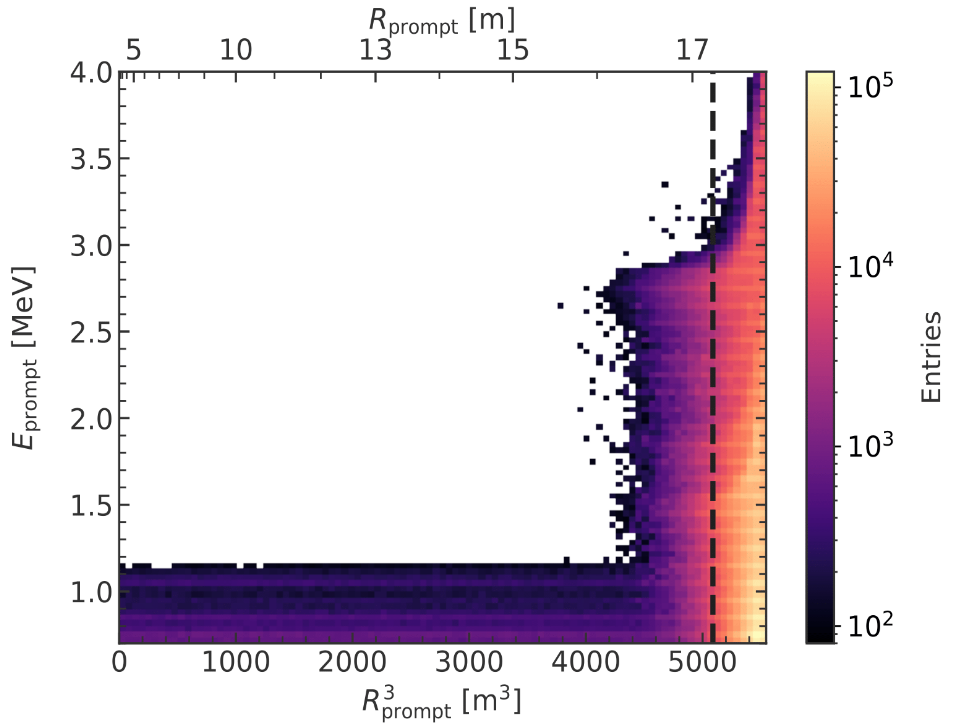
- For training and hyperparameter optimization, **balanced dataset is used** to prevent biases:
  - 15M of IBD pairs
  - 15M of accidental coincidences

20M for training, 5M for validation, 5M for testing

IBDs (signal): *Uniformly distributed in the detector*

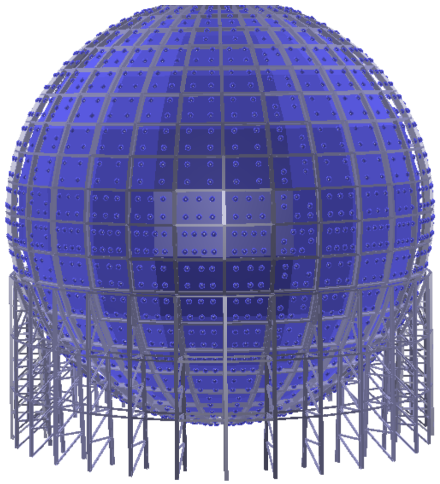


Accidentals (background): *Mostly at the detector edge*



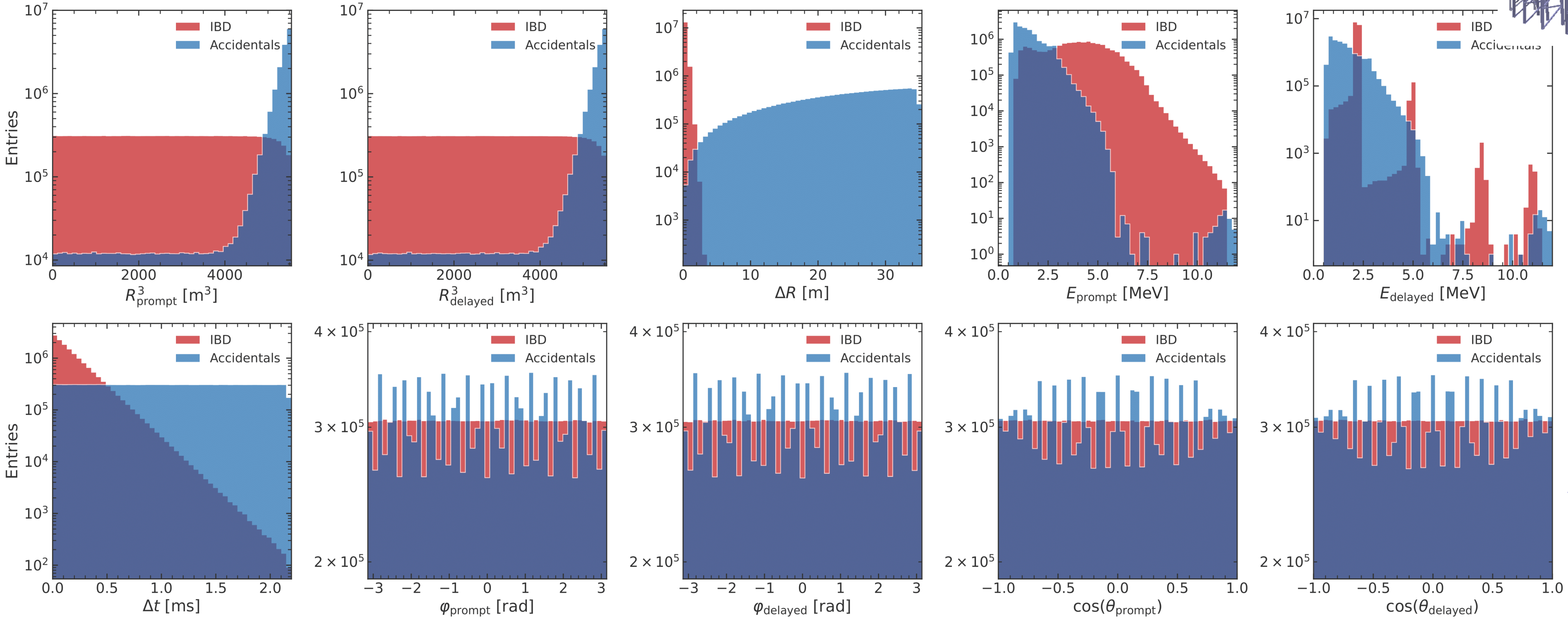
[1] arXiv:2405.18008
[2] JHEP11(2021)102

DATA DESCRIPTION: FEATURE DISTRIBUTIONS



10 energy and vertex related features:

$$R^3{}_p, R^3{}_d, \Delta R, \Delta t, Ep, E_d$$
$$\cos\theta_p, \cos\theta_d, \varphi_p, \varphi_d$$



Higher radioactivity at the edges from the stainless steel grid

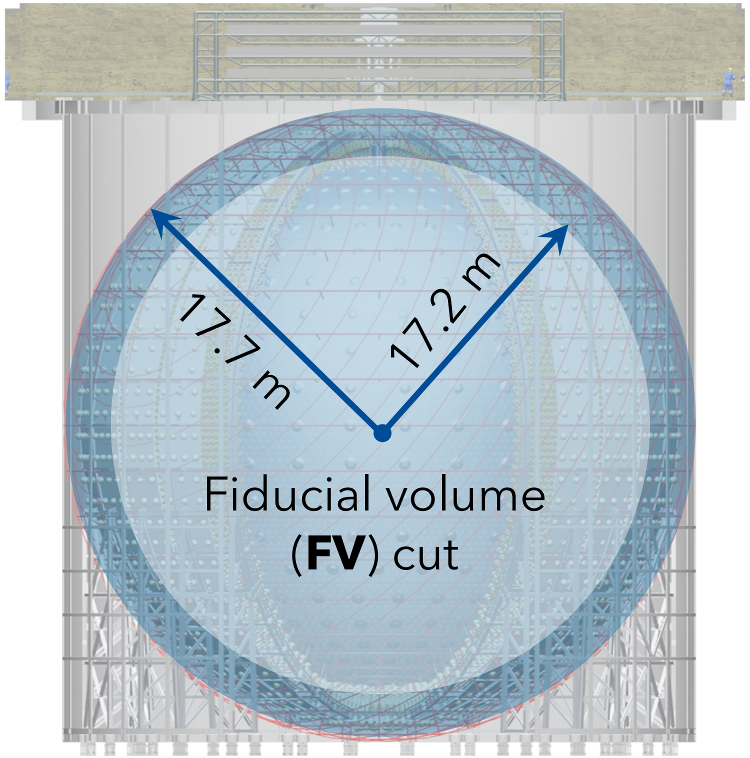
*The dataset was produced independently of the JUNO official software

BENCHMARK SELECTION: CUTS

✶ Benchmark for a machine learning approach → cut-based selection strategy from [1]

Independent cuts

		Efficiency
FV cut	$R < 17.2$ m	**91.7%**
Energy cut	$E_d \in (1.9, 2.5) \cup (4.4, 5.5)$ MeV $E_p \in (0.7, 12)$ MeV	**98.7%**
Vertex cut	$\Delta R < 1.5$ m	**99.0%**
Time cut	$\Delta t < 1$ ms	**99.4%**



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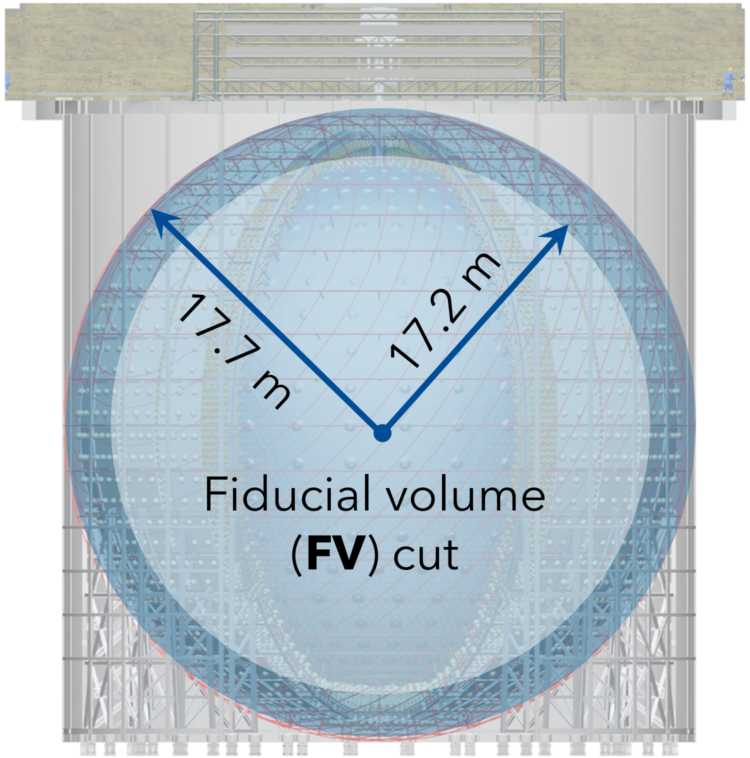

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Efficiency

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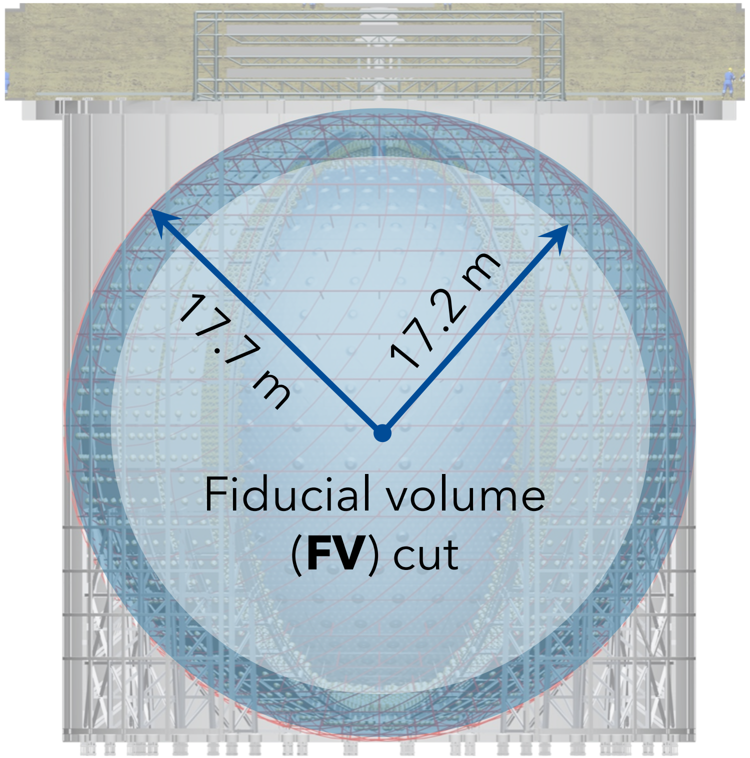
Combined 97.1%



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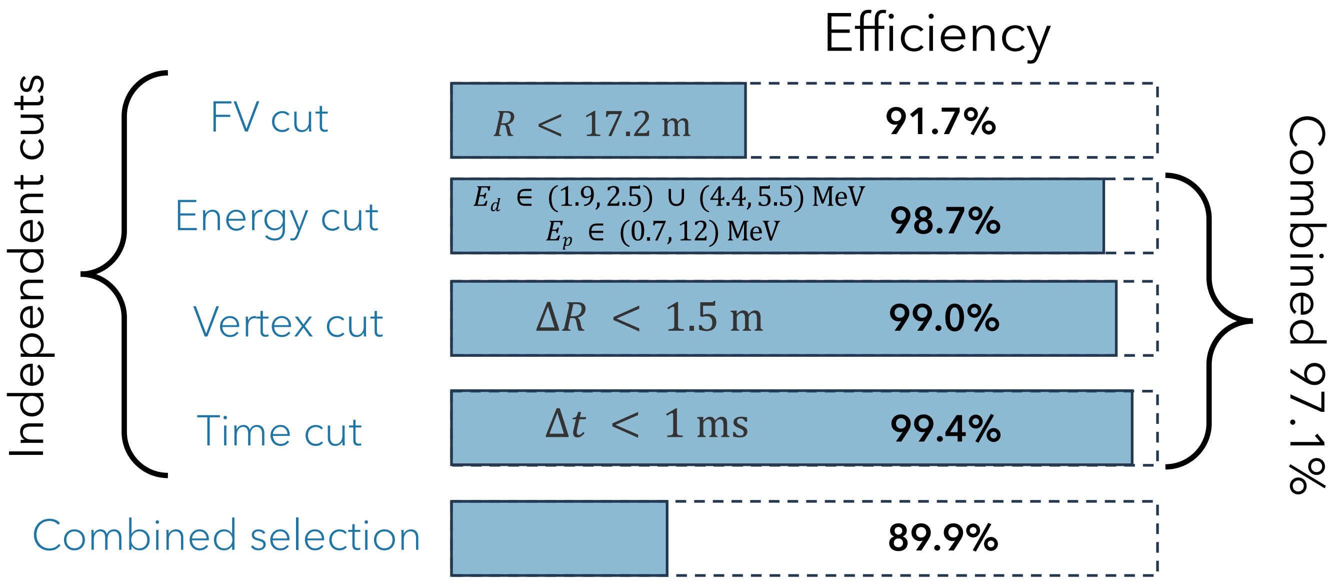
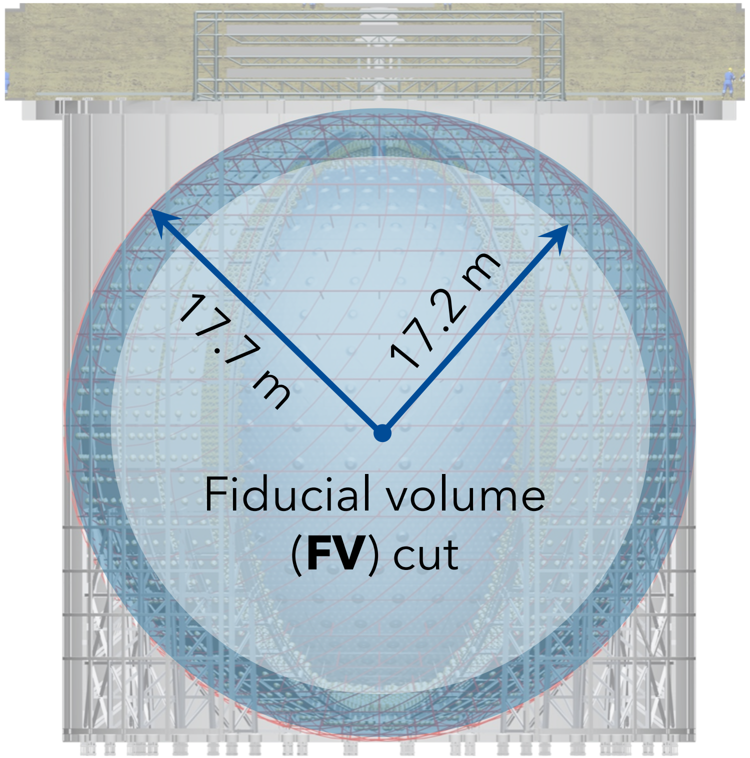
  - Can we **improve the overall efficiency**?





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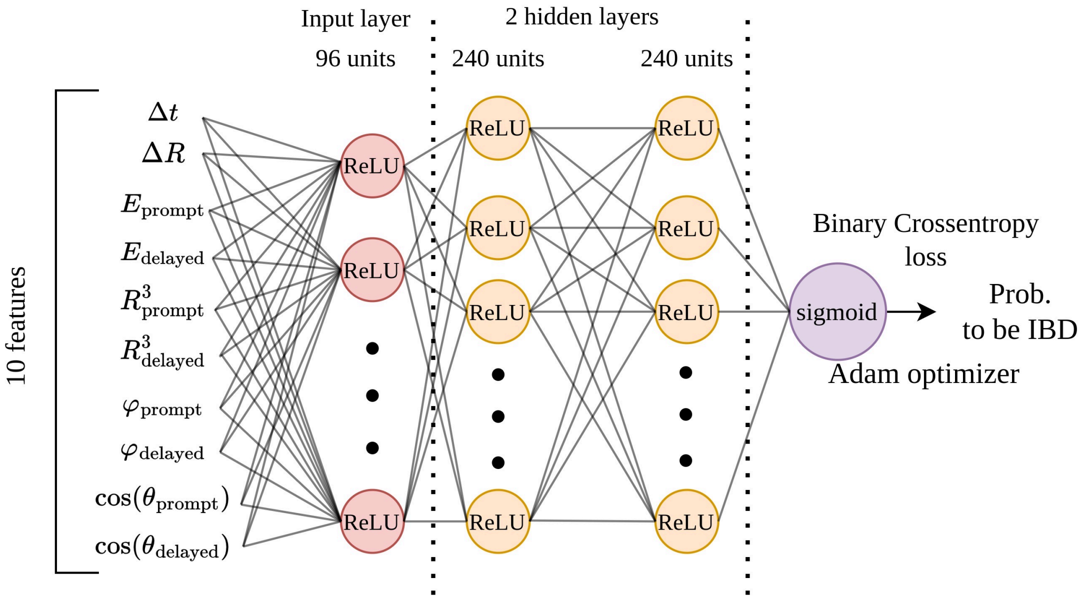
MACHINE LEARNING APPROACH

NEURAL NETWORK ARCHITECTURE

- ✶ Supervised classification problem
- ✶ Goal: **separate** between IBDs and accidentals
- ✶ Comprehensive **hyperparameter optimization** to find optimal number of layers, number of units in a layer, learning rate, etc., …

- ✶ 10 input features:
  - Time and vertex distance: $\Delta t, \Delta R$
  - Prompt and delayed energies: E_p, E_d
  - Distance from detector center: $R^3{}_p, R^3{}_d$
  - Angular variables: $\varphi_p, \varphi_d, \cos\theta_p, \cos\theta_d$

Optimized architecture: Fully Connected Neural Network



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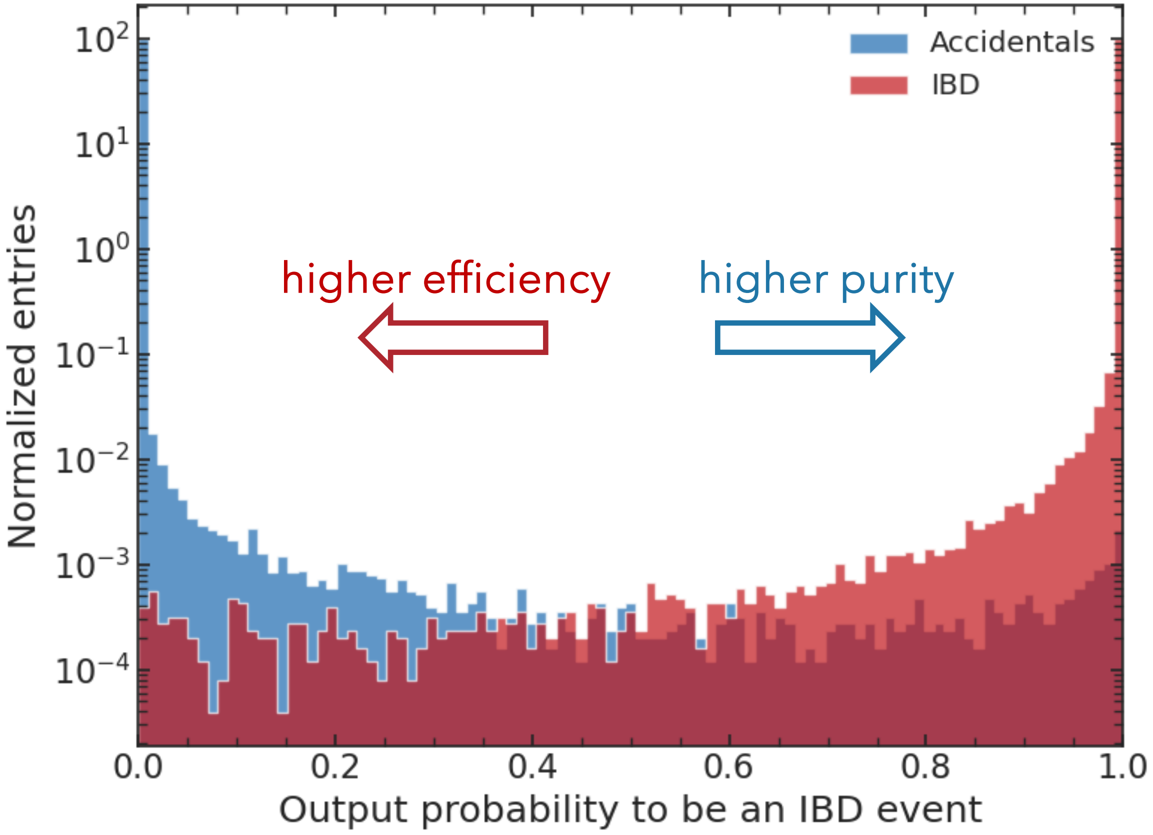
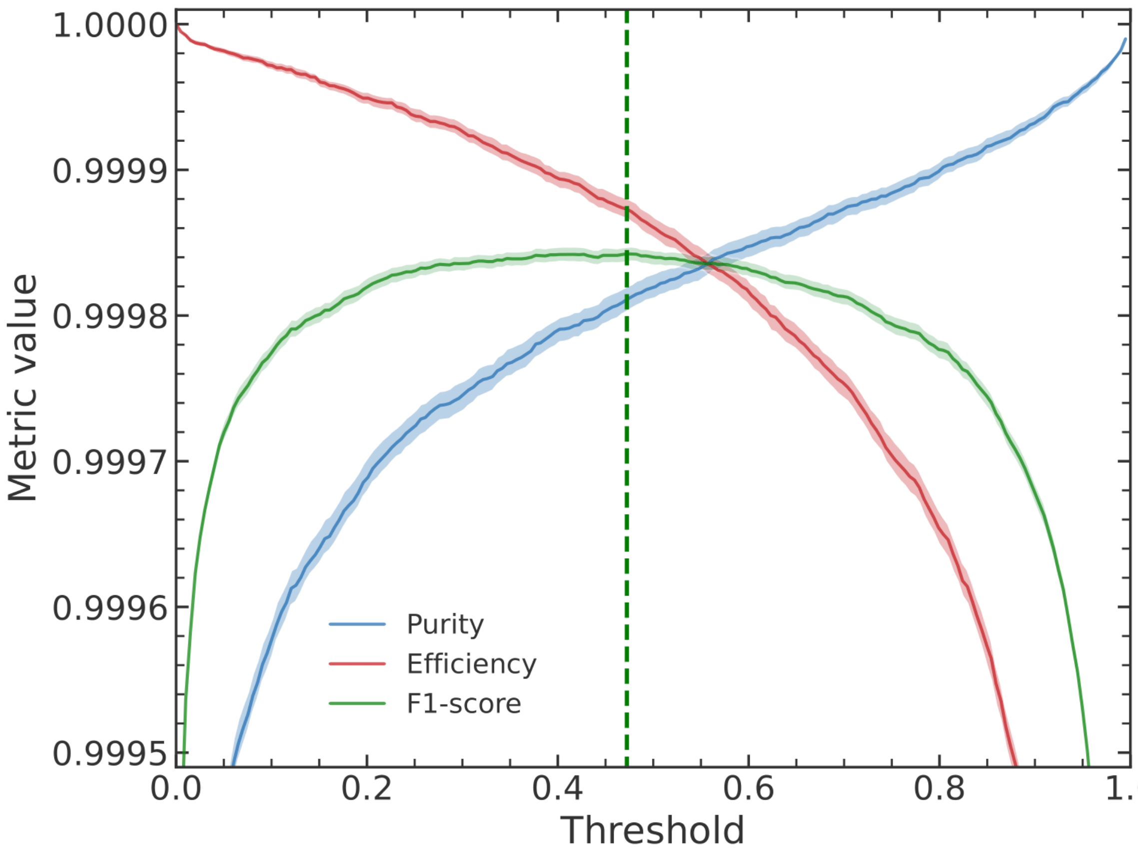
NEURAL NETWORK: A TUNABLE CLASSIFIER

- Output: **confidence score to be an IBD event**, from 0 to 1



NEURAL NETWORK: A TUNABLE CLASSIFIER

- ✶ Output: **confidence score to be an IBD event,** from 0 to 1
- ✶ **Threshold** to assign a class is **a tunable parameter**
- ✶ For different physics channels we can use:
    - same model
    - different thresholds
    - optimize the desired metric (efficiency or purity)



Balance purity and efficiency by maximizing the *harmonic mean* of efficiency and purity: **F1-score**

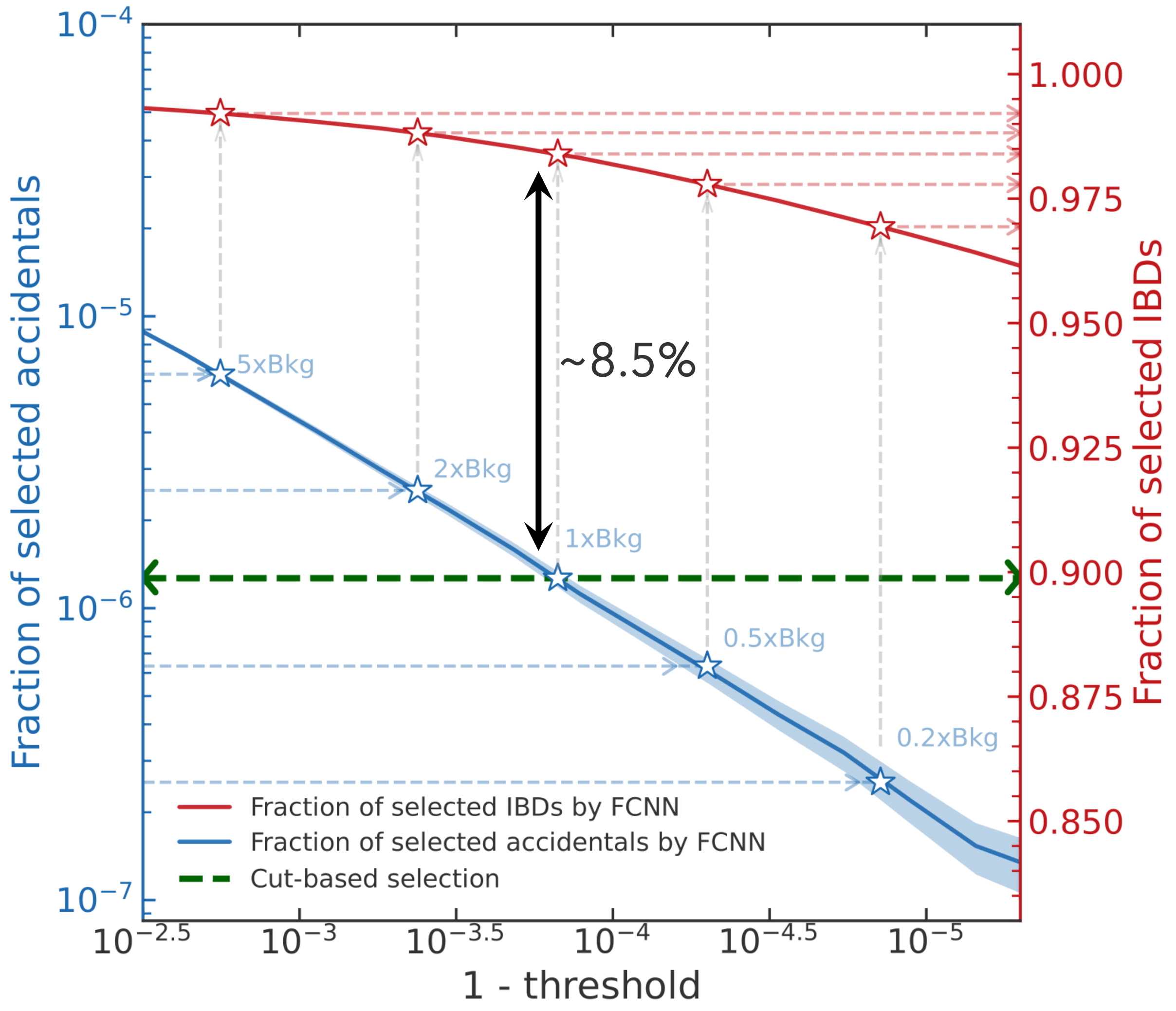
$$\text{F1-score} = 2 \cdot \frac{\text{purity} \cdot \text{efficiency}}{\text{purity} + \text{efficiency}}$$

NEURAL NETWORK: PERFORMANCE

- ✶ Model can be used **in the entire volume**, without fiducial volume cut

- ✶ Improvement of ~8.5% points in efficiency for the same background level as for the cuts*

Unbalanced dataset: 150M accidentals, 2.5M IBDs



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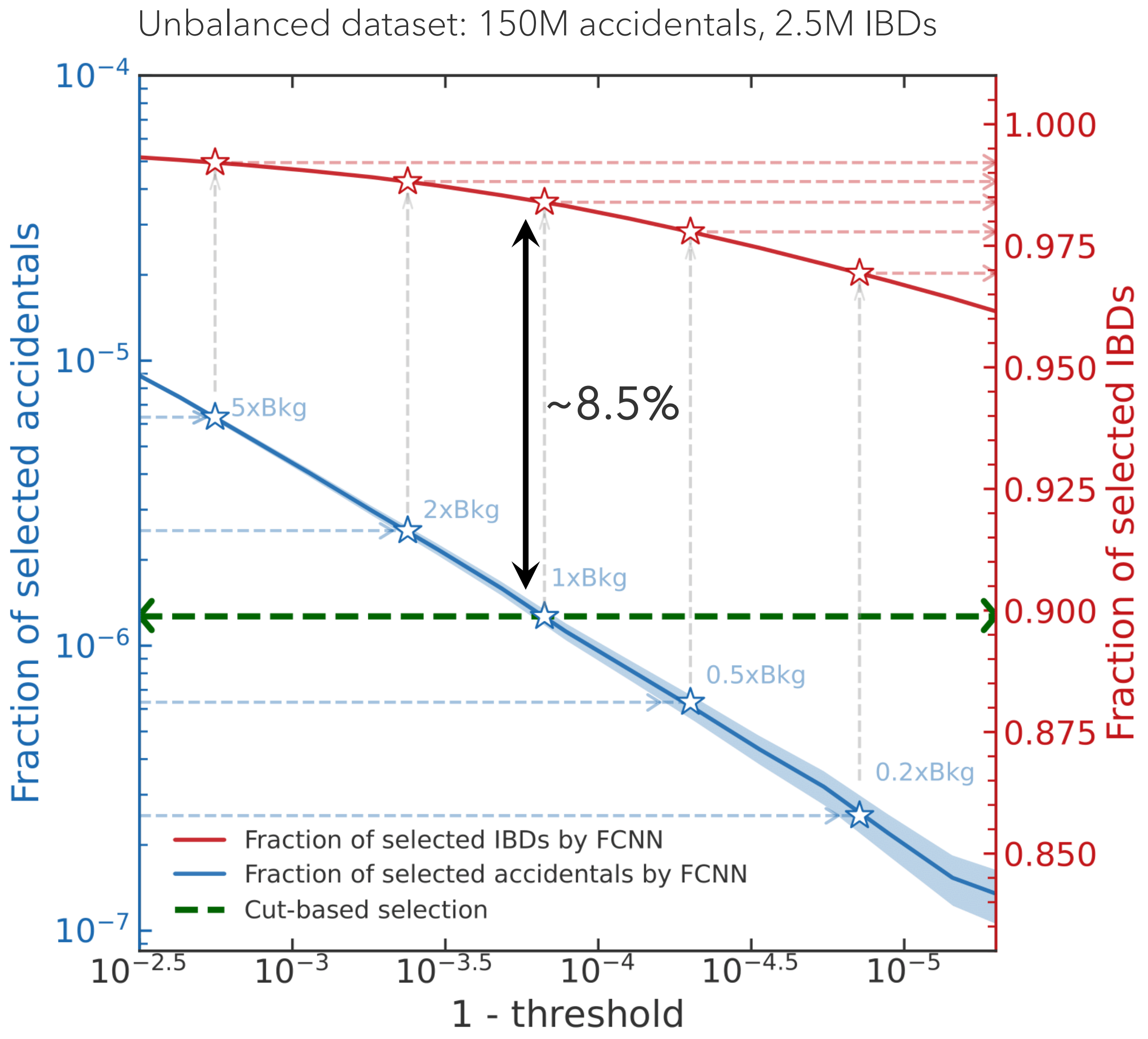
NEURAL NETWORK: PERFORMANCE

- Model can be used **in the entire volume**, without fiducial volume cut

- Improvement of ~8.5% points in efficiency for the same background level as for the cuts*

- Background can be further decreased, keeping higher efficiency

- Efficiency can be further increased, having higher residual background



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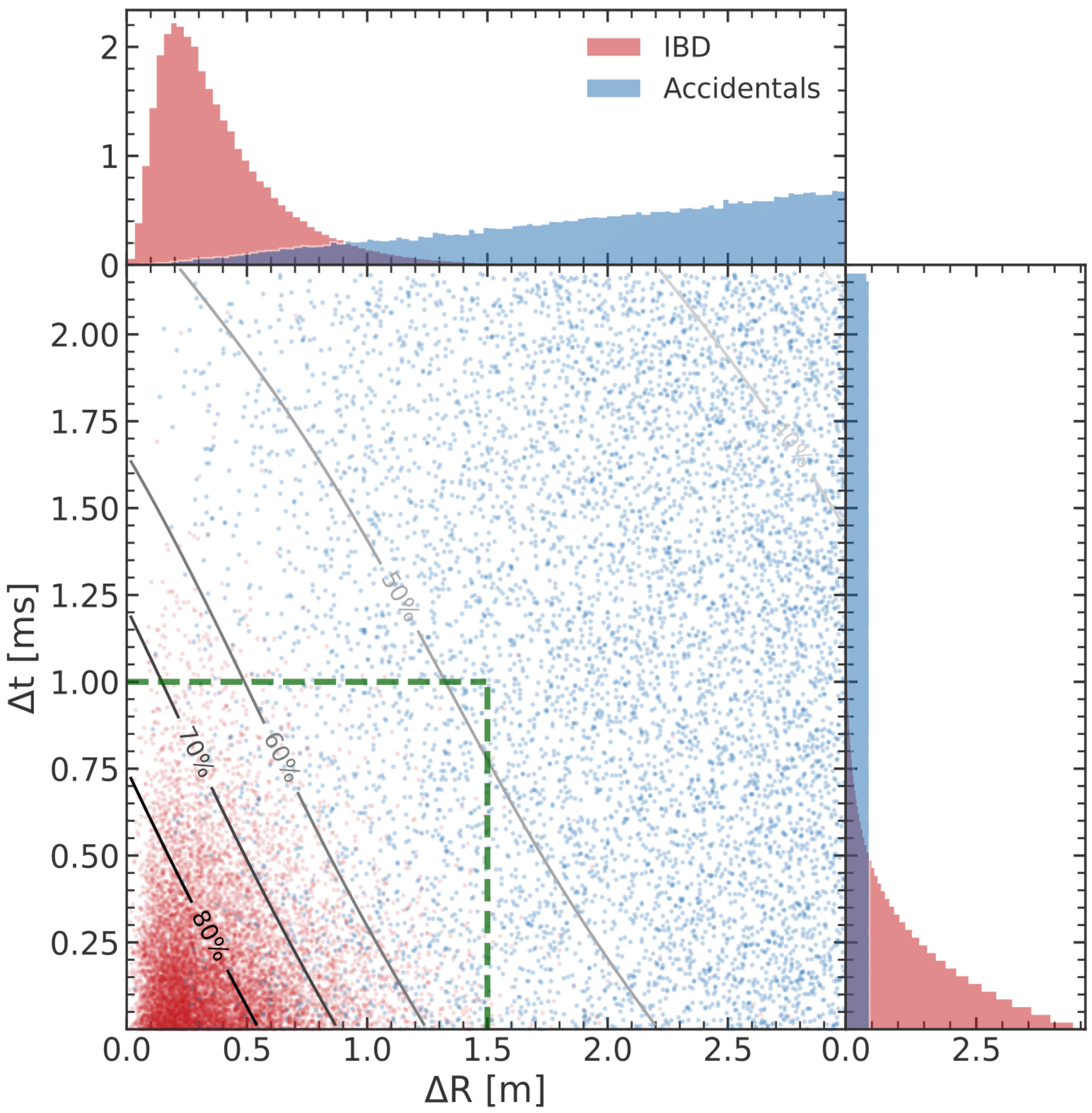
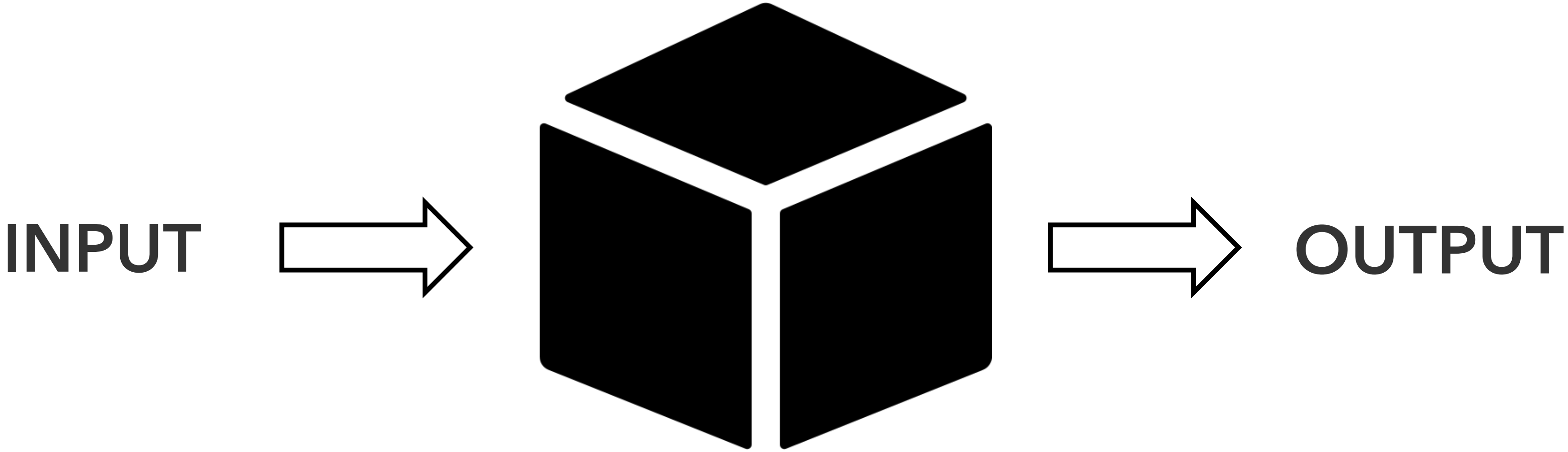
OPTIMIZATION OF IBD SELECTION CUTS

- ✶ Standard ΔR and Δt cuts are box-like
- ✶ ML model has learnt smoother decision boundary
  - Increased efficiency
  - Close-to-linear relation
  - Can be used to optimize selection criteria



INTERPRETABILITY

WHY INTERPRETABILITY?



- ✶ Hard to understand how and why a neural network made a decision → *Black box*

WHY INTERPRETABILITY?

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WHY INTERPRETABILITY?

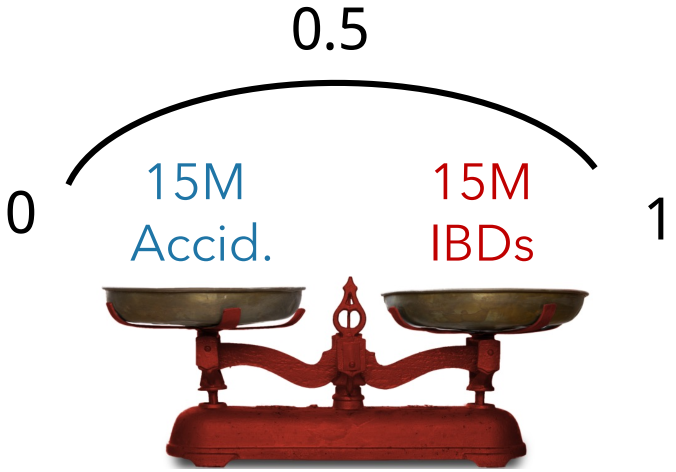
- ✶ Hard to understand how and why a neural network made a decision → ~~*Black box*~~
- ✶ Explainable AI: methods that allow users to comprehend results created by AI algorithms
- ✶ Goals:
    - **Ensure trust** in the model and its **transparency**
    - Identify features driving decision about classification
    - **Optimize and fine-tune** the cut-based selection strategy

INTERPRETABILITY AND SHAP VALUES

- SHAP (**SH**apley **A**dditive ex**P**lanations)
  - Calculate the contribution of each feature
  - Can be positive or negative
  - Show the **impact on predictions with respect to the average**

- Positive SHAP values → IBD class

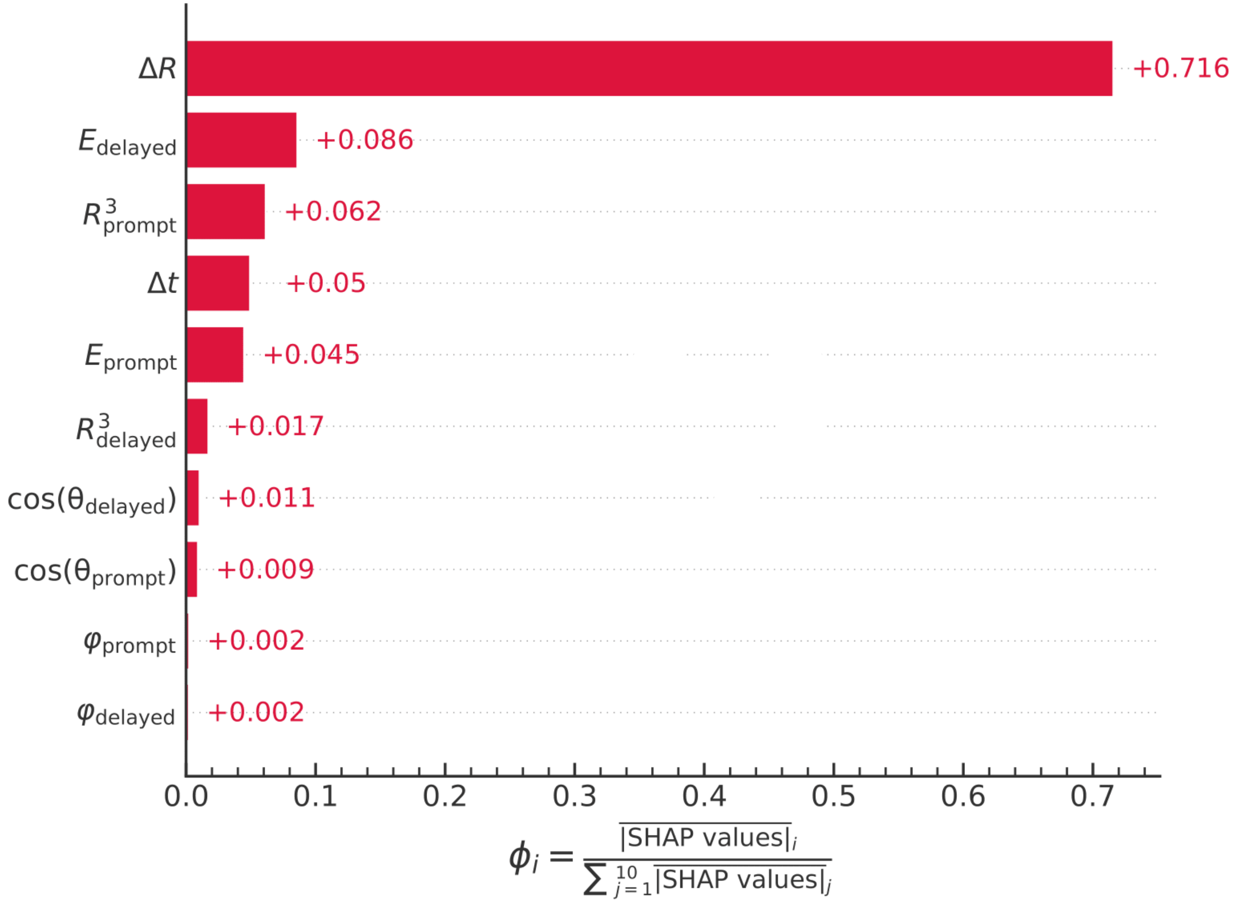
- Negative SHAP values → accidentals class



GLOBAL EXPLANATIONS

What features are the most important for the model's predictions on average?

- Global explanations: **summarized impact** of a specific feature
- Most important feature is distance between prompt and delayed candidates' vertices ΔR
- Energy of delayed candidate has **the next stronger** discriminative power
- $R^3{}_{\text{prompt}}$, $R^3{}_{\text{delayed}}$ provide additional information, especially at the edges
- Δt in top 4 features for importance



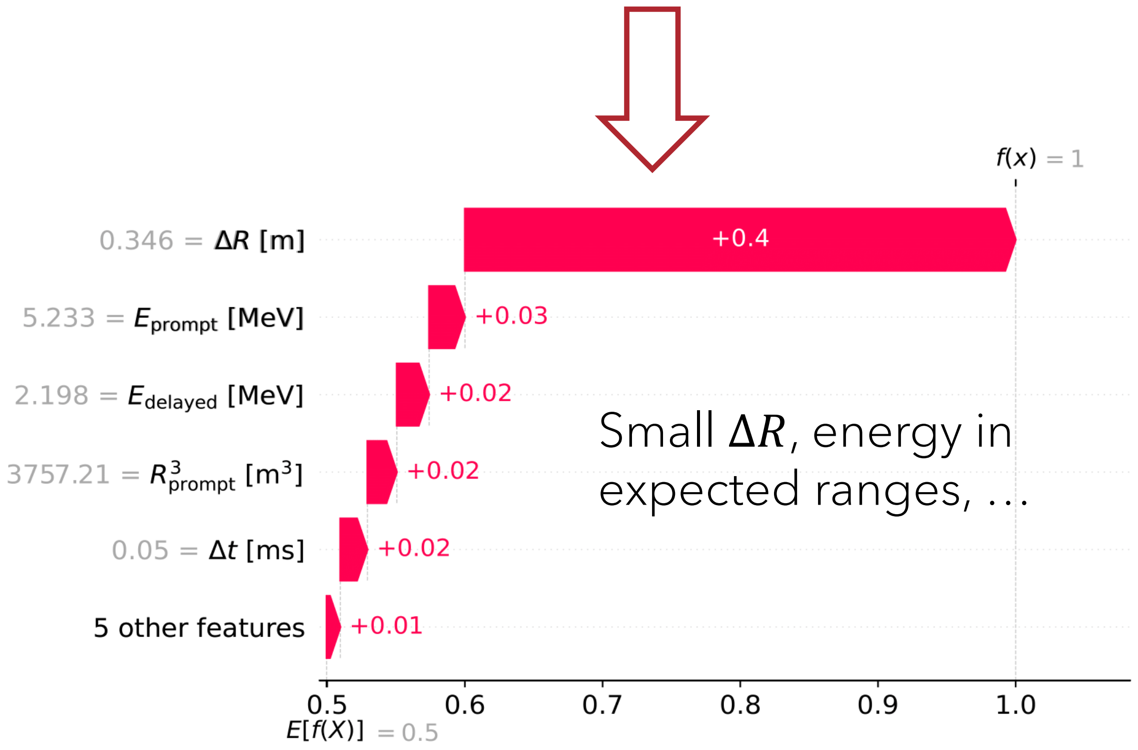
LOCAL EXPLANATIONS – GOOD CLASSIFICATION

Why did the model make this prediction for this specific data point?

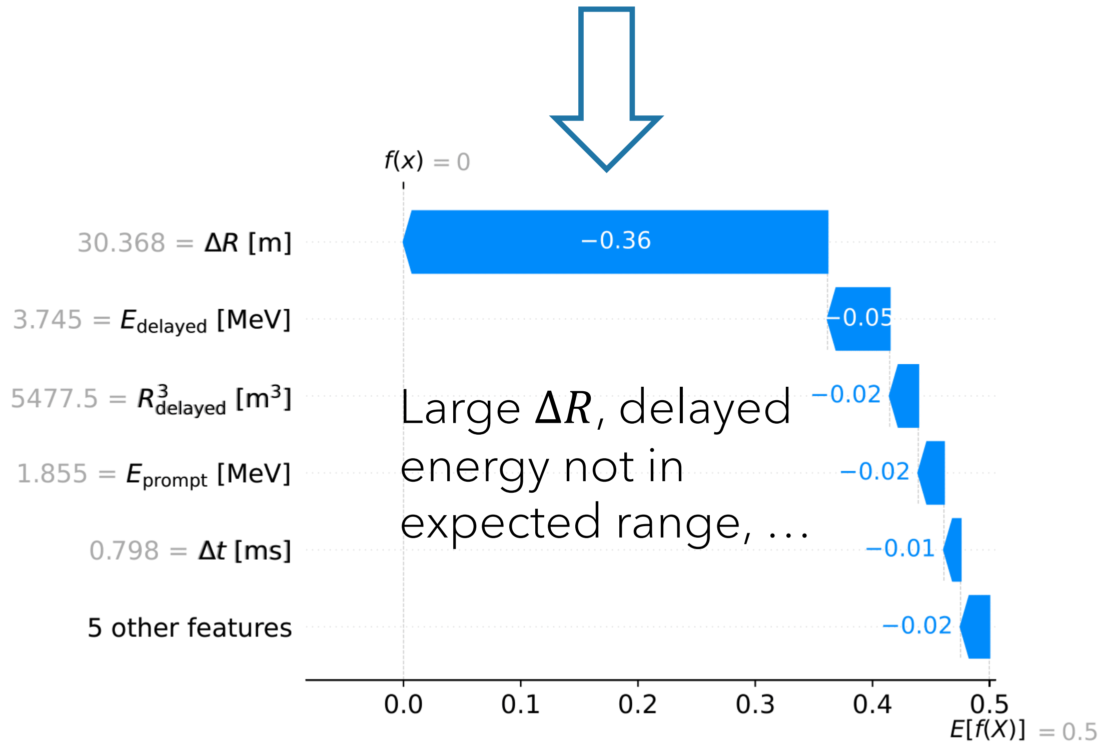
- ✶ Local explanations focus on an individual event and provide features' importances for a specific instance

- ✶ **Example of good classification**: typical correctly classified events

True positives (IBDs)



True negatives (accidentals)

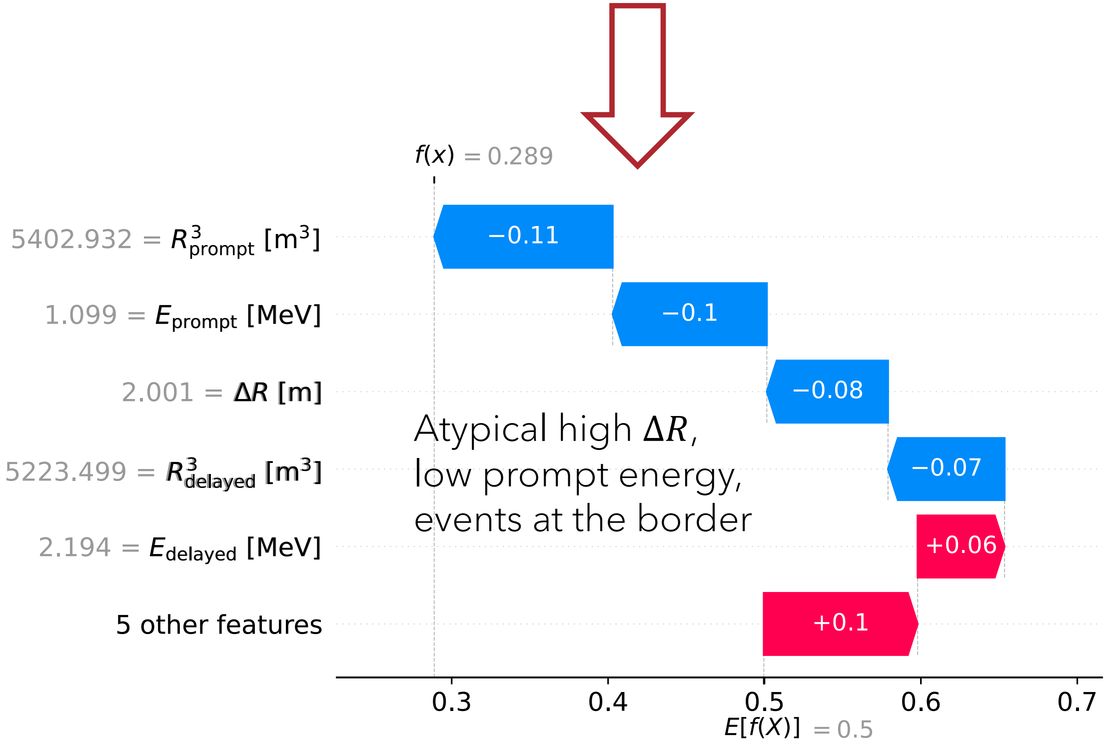


LOCAL EXPLANATIONS – MIS-CLASSIFICATION

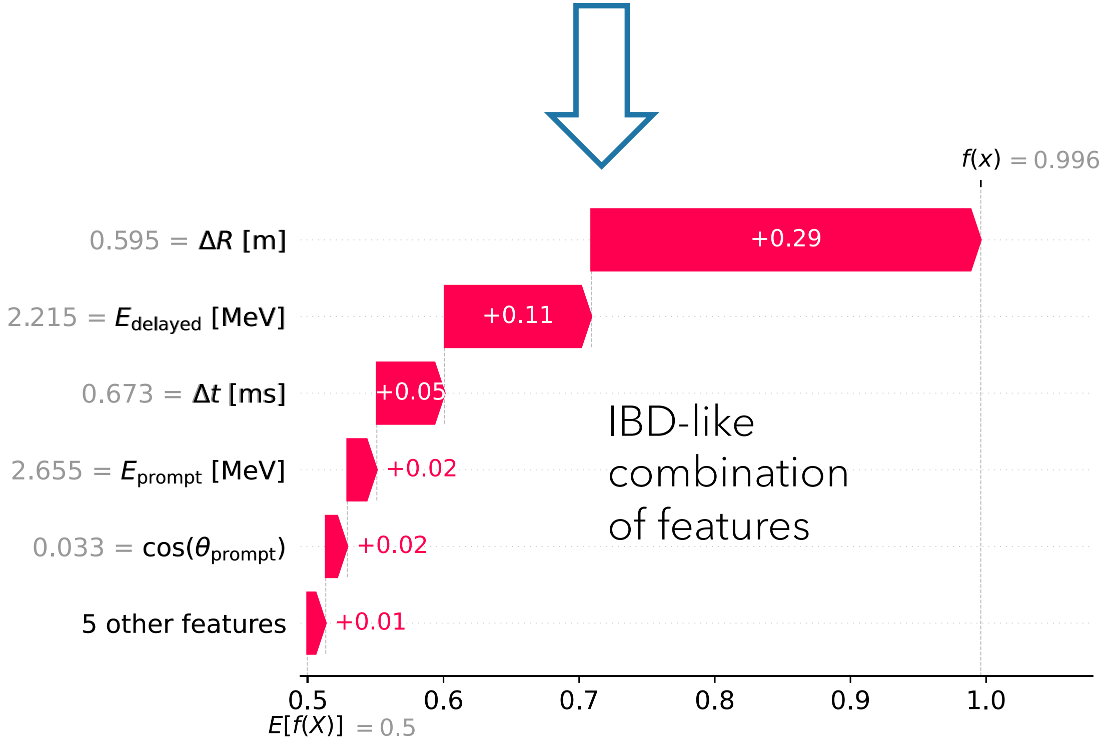
- Local explanations focus on an individual event and provide features' importances for a specific instance

- **Example of mis-classification**: wrongly classified events

IBDs classified as accidentals



Accidentals classified as IBDs

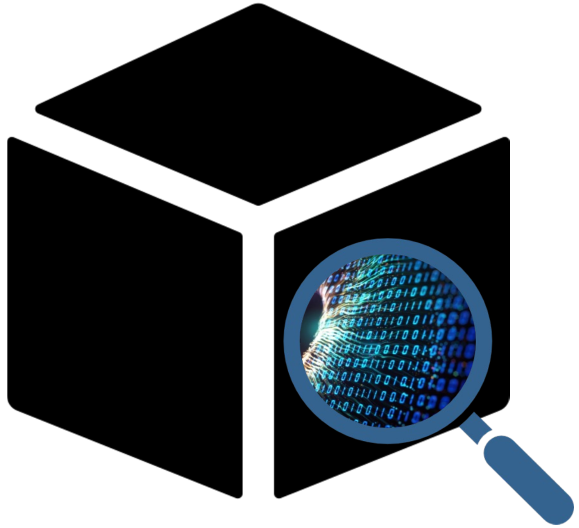


CONCLUSIONS

- ✶ The main task of a **selection algorithm** is to distinguish between two classes: **reactor antineutrino events and accidental coincidences** (mainly from radioactivity)

- ✶ Introduced a fully-connected **neural network** as IBD-accidentals classifier
  - Can be applied as **a proxy to improve the cut-based selection**
  - **Provides higher efficiency** than the cut-based selection within both fiducial volume and the entire volume
  - Provides **higher efficiency** for **higher purity level**

- ✶ Interpretability analysis
  - Ensures trust in the model predictions → ~~*Black box*~~
  - Identify features driving decision about classification
  - **Offers valuable insights** into the model behavior



BACKUP

LS-BASED REACTOR NEUTRINO EXPERIMENTS

- ✶ The medium of choice for most reactor neutrino experiments has been **liquid scintillator (LS)**
- ✶ Organic liquid scintillator detectors:
  - High light yield → energy resolution
  - Large proton abundance → antineutrino target
  - Large volume → compensate small cross section
  - Doping capabilities → improve signal-background discrimination

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Detector design is driven by ambitious physics goals:

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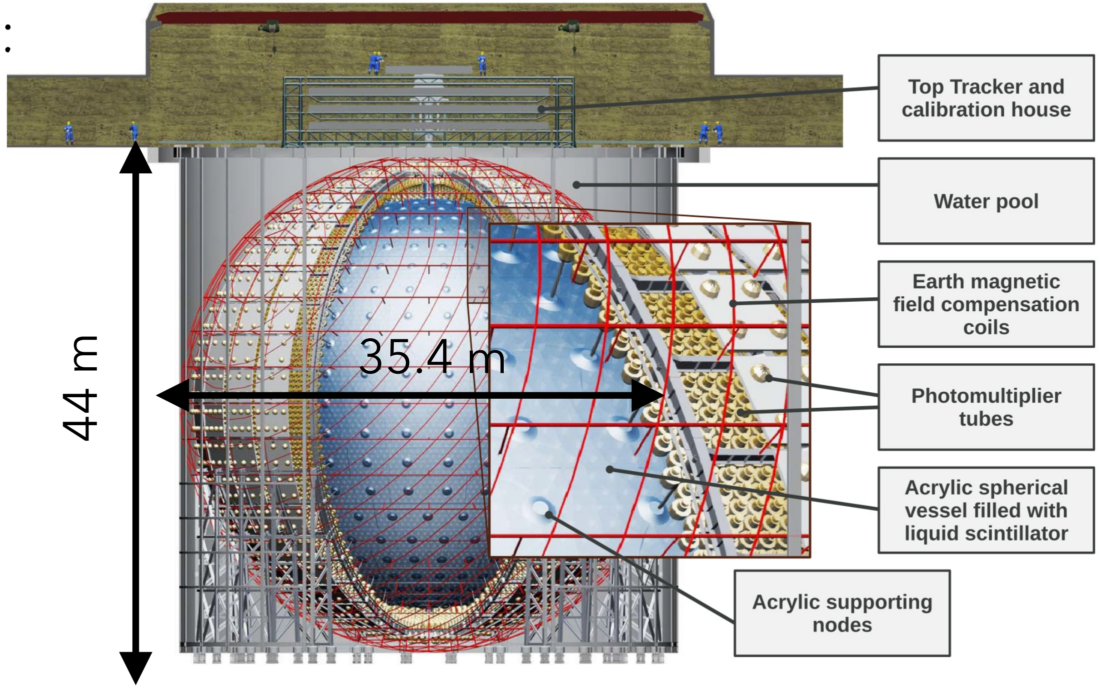

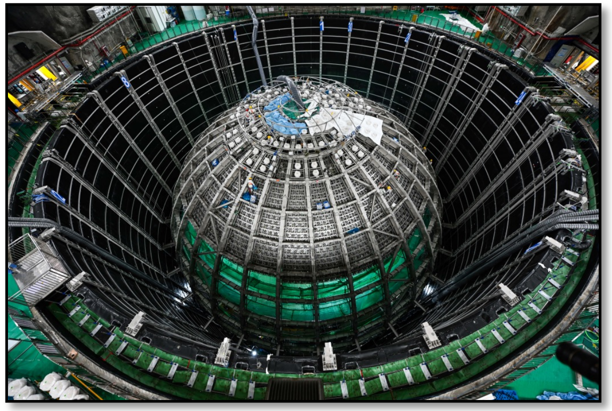

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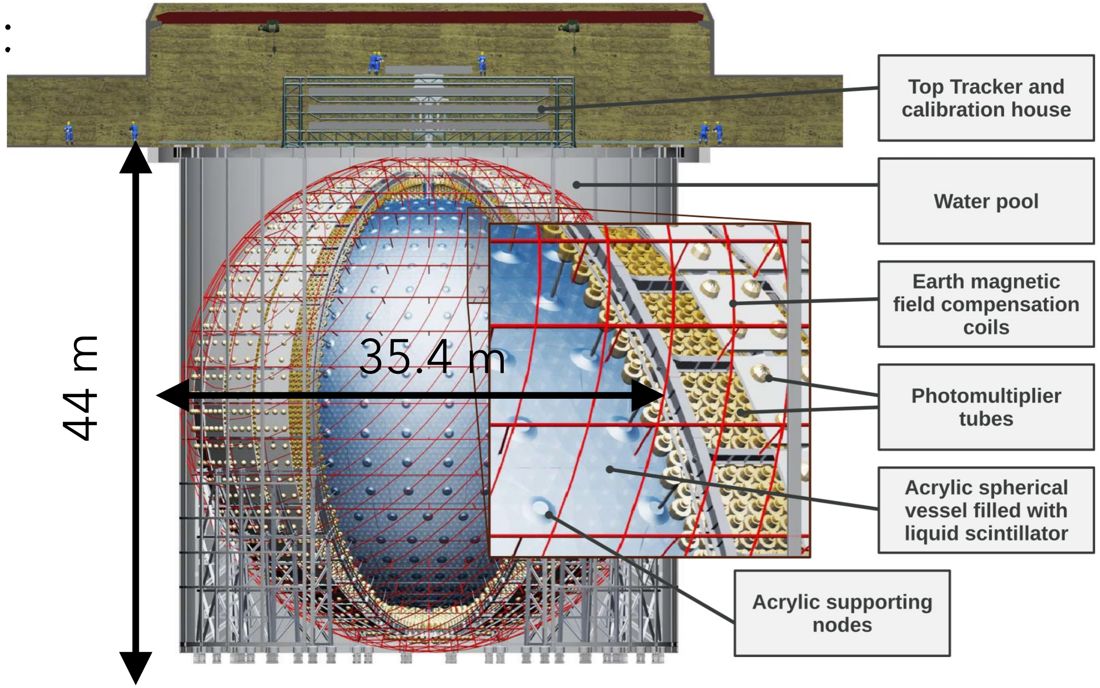
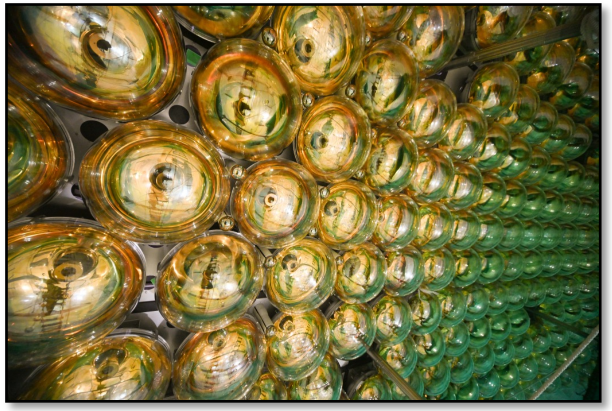
  - ✓ High photon yield, highly transparent LS
  - ✓ Total photo-coverage ≈ 78%
- ✶ Control of non-linear energy scale within 1%
  - ✓ Comprehensive calibration program
- ✶ Low background
  - ✓ 650 m underground
  - ✓ LS purification system and material screening
  - ✓ Efficient veto systems





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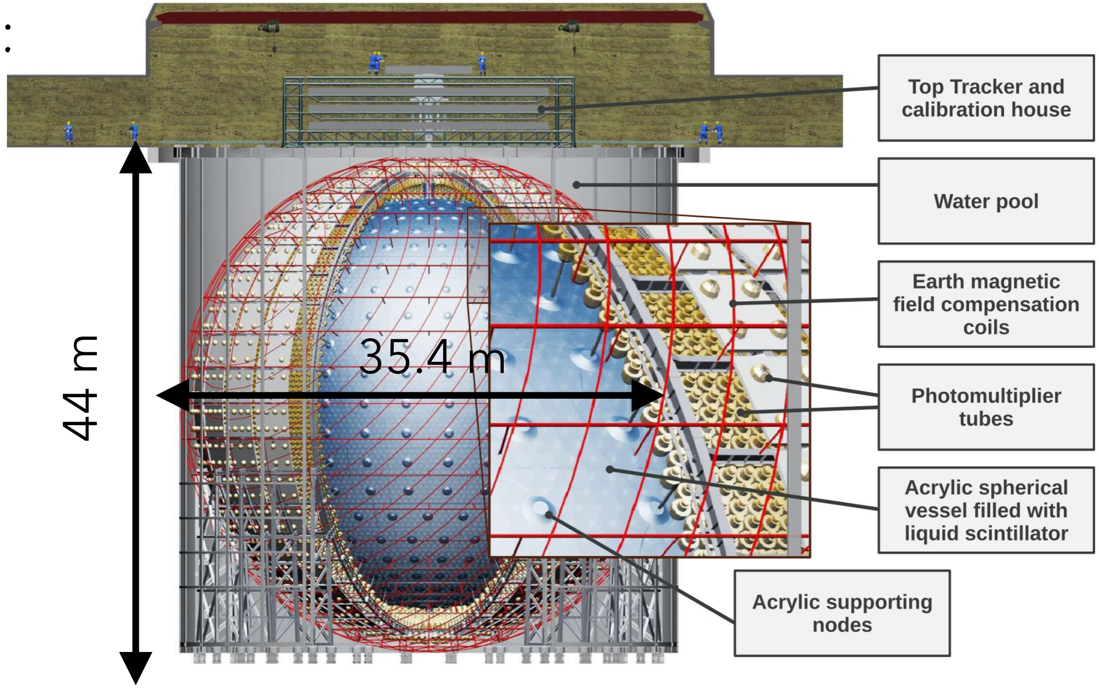
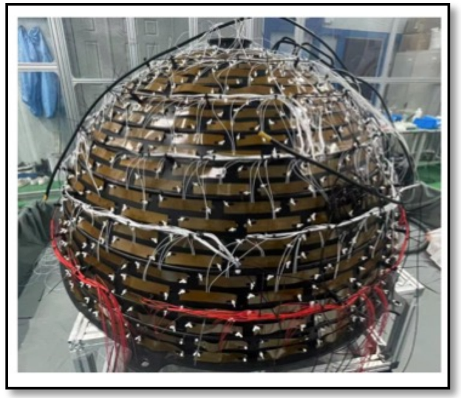
- ✶ Accurate knowledge of reactor spectra
  - ✓ Satellite near detector: **Taishan Antineutrino Observatory (TAO)** at 44 m from Taishan reactor





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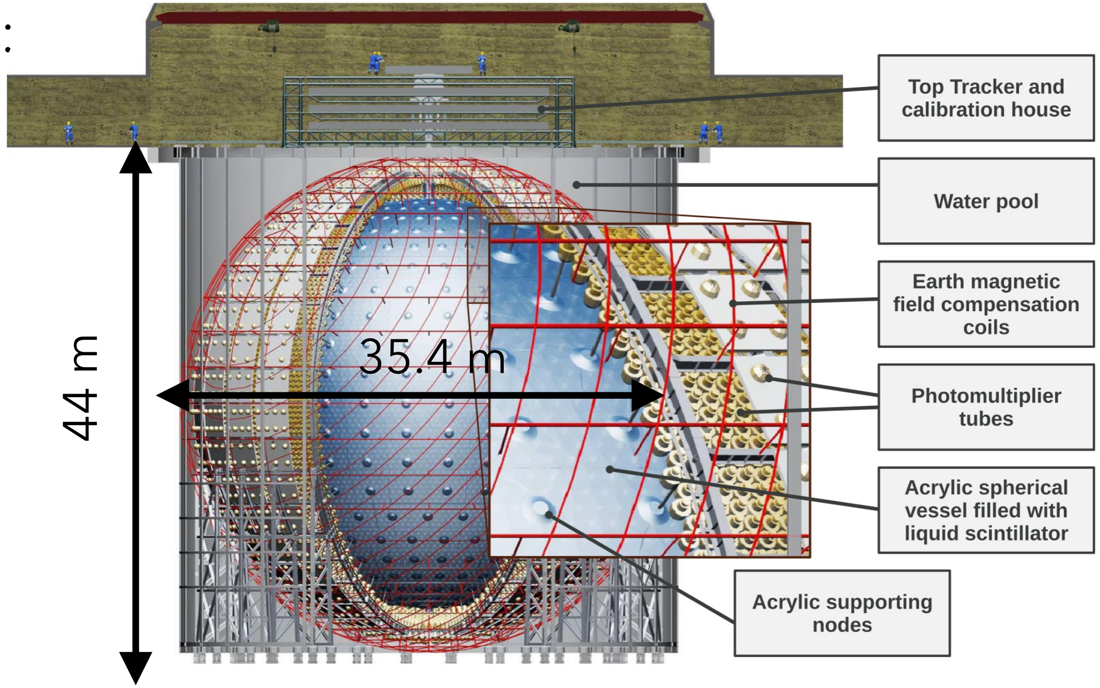

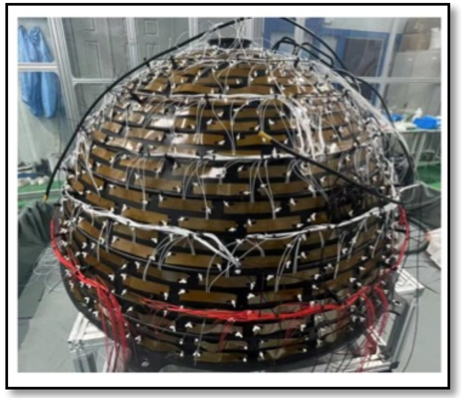

DETECTOR RESPONSE: WHAT JUNO MEASURES

[Chinese Phys. C 46 123001]

$E_\nu \xrightarrow{\textit{Interaction}} E_{\mathrm{dep}} \xrightarrow{\textit{Light emission}} E_{\mathrm{vis}} \xrightarrow{\textit{Light detection}} E_{\mathrm{rec}}$

Antineutrino energy	Deposited energy	Visible energy	Reconstructed energy

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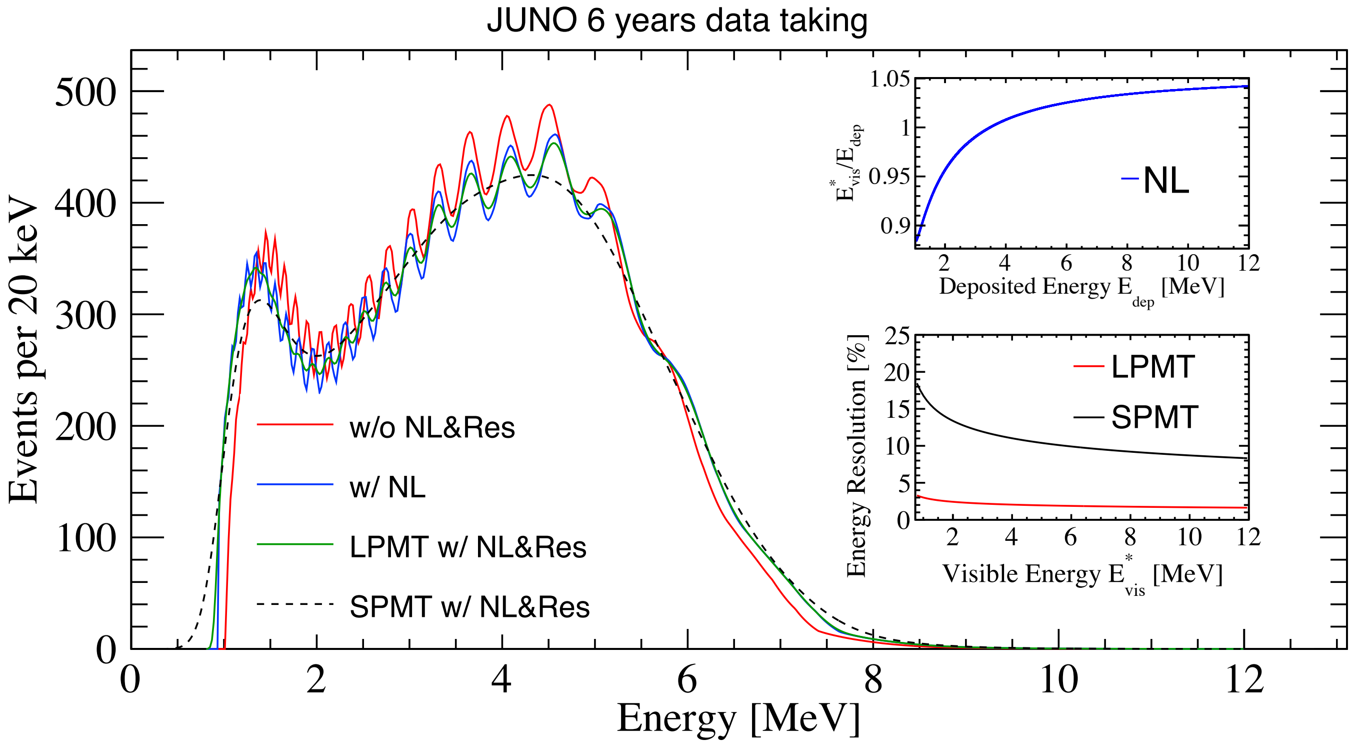


1. IBD reaction and cross section, e^+ deposited energy

$$E_{\text{dep}} \simeq E_{\bar{\nu}_e} - 0.782\,\text{MeV}$$

2. Liquid scintillator non-linearity (NL), visible energy ∝ detected photoelectrons

$$E_{\text{vis}} = f_{\text{LSNL}}(E_{\text{dep}}) \cdot E_{\text{dep}}$$

3. Energy resolution (Res)

$$\frac{\sigma_{E_{\text{rec}}}}{E_{\text{vis}}} = \sqrt{\left(\frac{a}{\sqrt{E_{\text{vis}}}}\right)^2 + b^2 + \left(\frac{c}{E_{\text{vis}}}\right)^2}$$

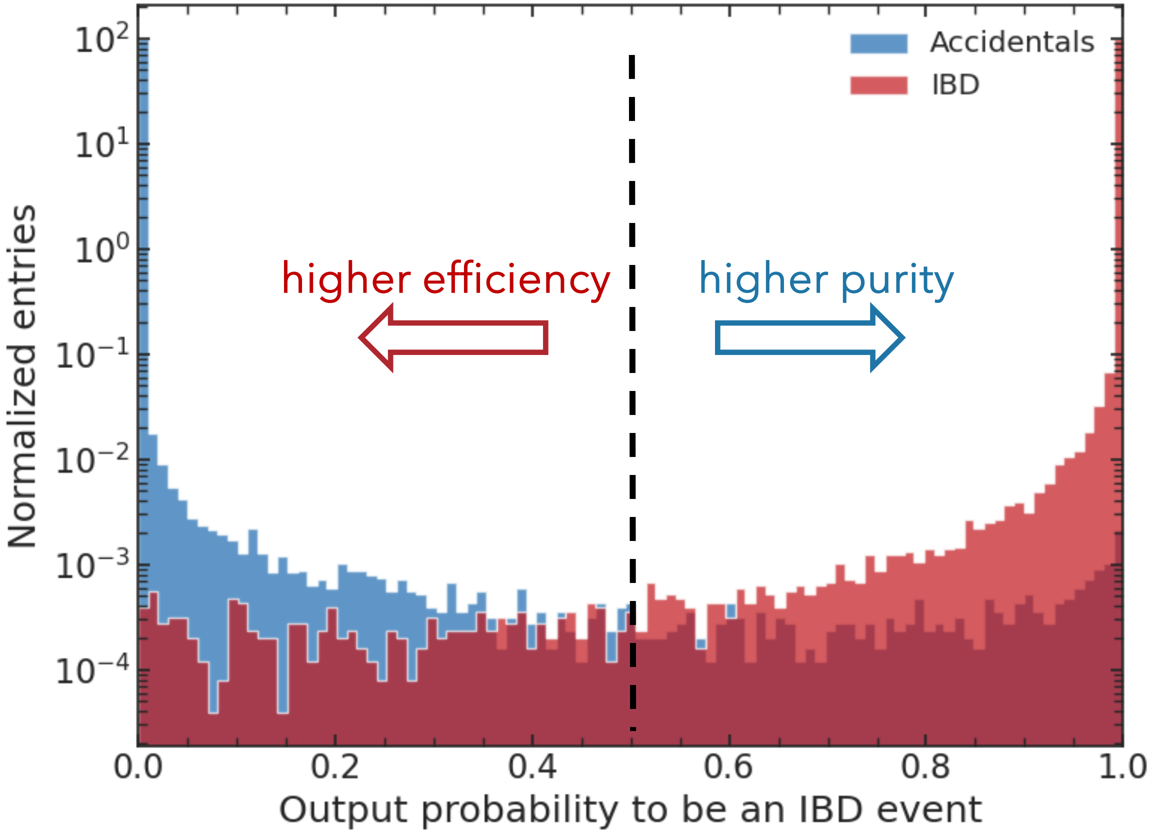
NEURAL NETWORK: A TUNABLE CLASSIFIER

✶ Output: **confidence score to be an IBD event,** from 0 to 1

✶ **Threshold** to assign a class is **a tunable parameter**

✶ For different physics channels we can use:

- same model
- different thresholds
- optimize the desired metric (efficiency or purity)



Balance purity and efficiency by maximizing the *harmonic mean* of efficiency and purity: F1-score

$$\text{F1-score} = 2 \cdot \frac{\text{purity} \cdot \text{efficiency}}{\text{purity} + \text{efficiency}}$$

NEURAL NETWORK: HYPERPARAMETER OPTIMIZATION

Hyperparameter	*Search space and **selected hyperparameter***
Units in input layer	[16, 256]: **96**
Units in hidden layers	[16, 256]: **240**
Number of hidden layers	[1, 10]: **2**
Activation	**ReLU**, Leaky ReLU, SiLU, PReLU, Tanh
Optimizer	**Adam**, SGD, RMSprop
Learning rate	$[10^{-5}, 10^{-1}]$: $\mathbf{3.5 \cdot 10^{-4}}$
Scheduler type	Exponential, ReduceOnPlateau, **CosineAnnealing**, None
Layer weights initialization	xavier uniform, xavier normal, **orthogonal**, normal, uniform
Batch normalization	True, **False**
Batch size	[128, 2048]: **1024**

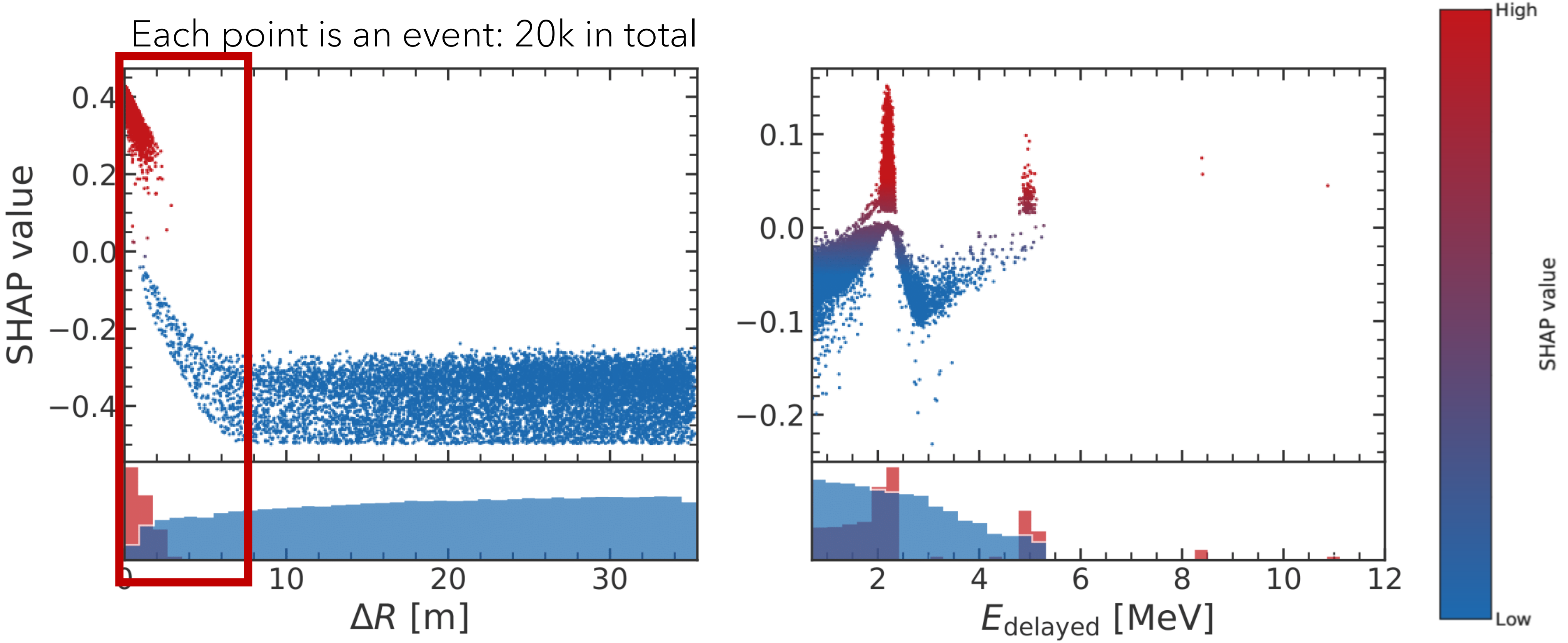
Table 1: Hyperparameter search space for FCNN. Selected hyperparameters are highlighted in bold.

NEURAL NETWORK: PERFORMANCE

Approach	*Volume*	*Efficiency*				
		0.2×Bkg	0.5×Bkg	1×Bkg	2×Bkg	5×Bkg
BDT	Full detector volume: $R < 17.7$ m	98.38%	98.81%	**99.02**%	99.19%	99.39%
	$R < 17.2$ m	91.58%	91.62%	**91.63**%	91.64%	91.64%
FCNN	Full detector volume: $R < 17.7$ m	96.94%	97.79%	**98.40**%	98.82%	99.21%
	$R < 17.2$ m	91.53%	91.60%	**91.63**%	91.64%	91.64%
Cuts	$R < 17.2$ m	—	—	89.90%	—	—

GLOBAL EXPLANATIONS FOR TOP FEATURES

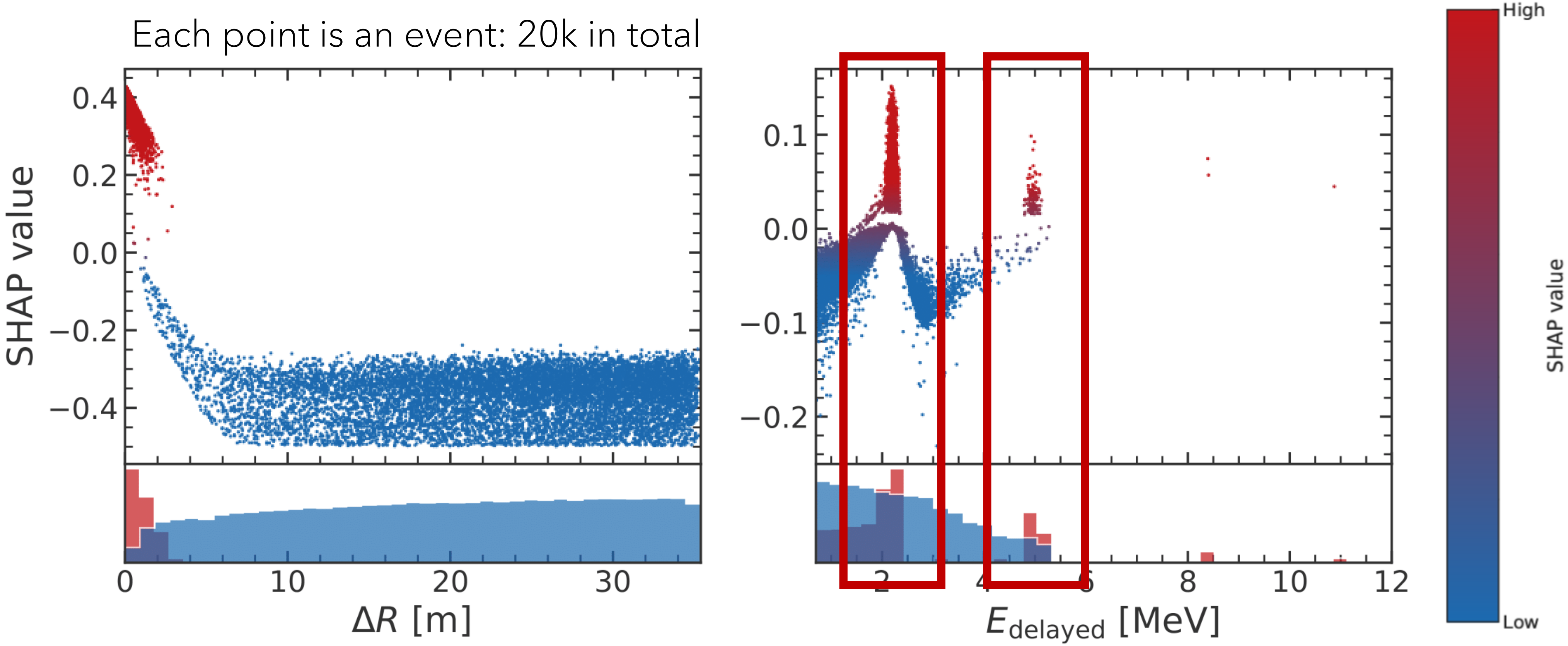
- Top-2 features distributions and SHAP values
- Small values of ΔR are very likely related to an IBD event



GLOBAL EXPLANATIONS FOR TOP FEATURES

- Top-2 features distributions and SHAP values
- Small values of ΔR are very likely related to an IBD event
- E_{delayed} has a clustered structure related to specific isotope on which **neutron** was captured

Each point is an event: 20k in total



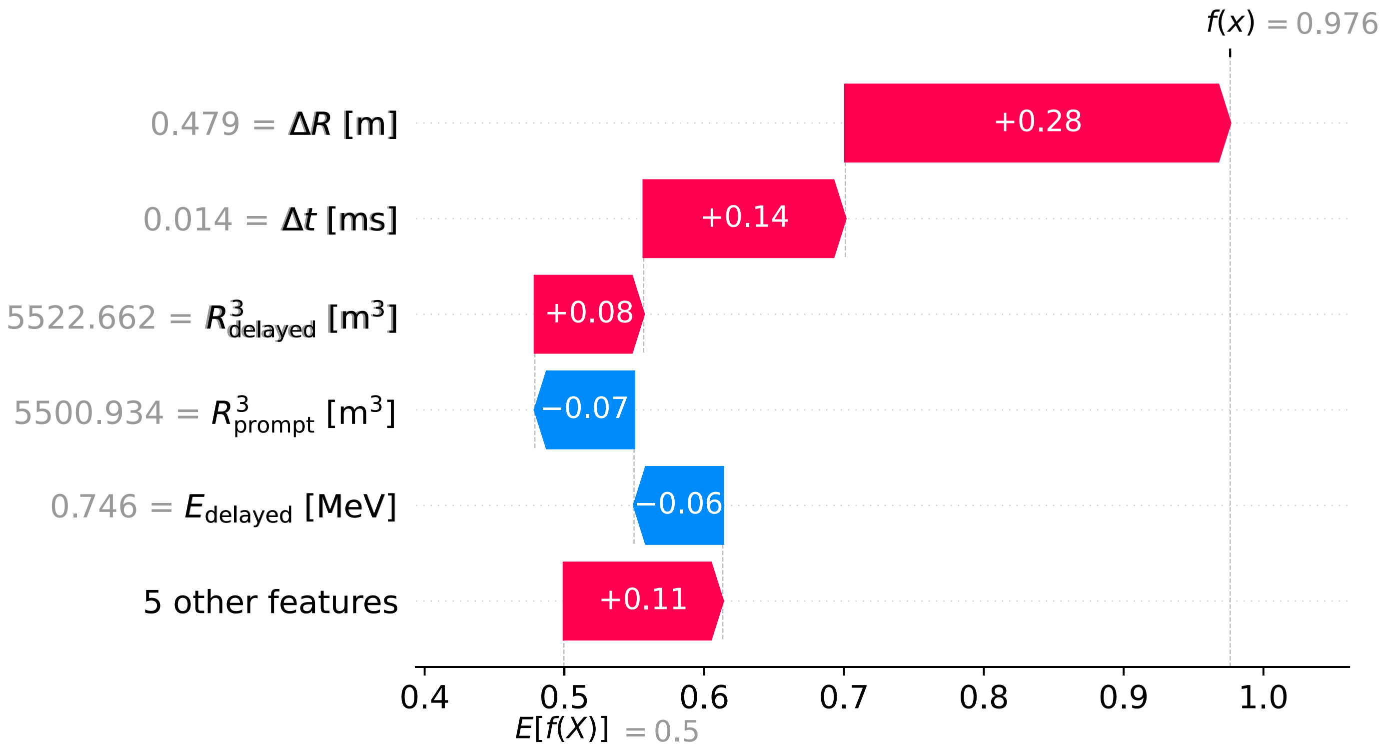
LOCAL EXPLANATIONS – GAMMA LEAKAGE

- Gamma produced by neutron capture escaping the target before depositing whole energy → gamma leakage

- Both prompt and delayed events occurred outside the FV

- This candidate pair would be **discarded** by cut-based selection → low E_{delayed} and FV cut

- NN classifies this as an IBD event based on the combination of other features → increase in efficiency ☺



INTERPRETABILITY AND SHAP VALUES

- SHAP (SHapley Additive exPlanations)
  - Calculate the contribution of each feature
  - Can be positive or negative
  - Show the **impact on predictions with respect to the average**

- Positive SHAP values → IBD class

- Negative SHAP values → accidentals class