

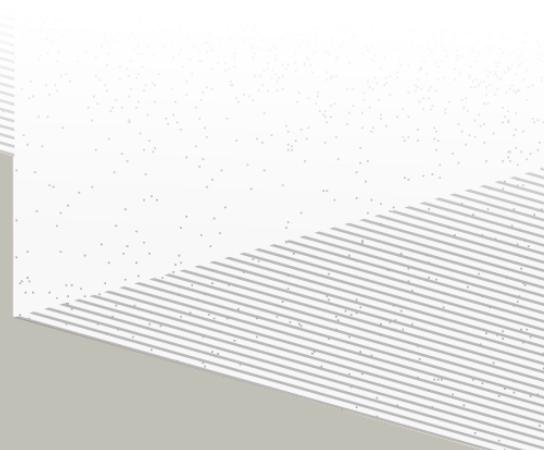
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Par

Léonard Imbert

**Precision measurement of solar neutrino oscillation parameters
with the JUNO small PMTs system and test of the unitarity of the
PMNS matrix**

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Rapporteurs avant soutenance :

Someone	Very high position, Somewhere
Someone else	Another high position, Somewhere else

Composition du Jury :

Président :	Jacques Chirac	French president, France
Examinateurs :	Yoda	Master, Dagobha
Dir. de thèse :	Frédéric Yermia	Professeur, Université de Nantes
Co-dir. de thèse :	Benoit Viaud	Chargé de recherche, CNRS

Invité(s) :

Victor Lebrin Docteur, CNRS/SUBATECH

³ Contents

⁴	Contents	¹
⁵	Remerciements	⁵
⁶	Introduction	⁷
⁷	1 Neutrino physics	⁹
⁸	1.1 Standard model	⁹
⁹	1.1.1 Limits of the standard model	⁹
¹⁰	1.2 Historic of the neutrino	⁹
¹¹	1.3 Oscillation	⁹
¹²	1.3.1 Phenomologies	⁹
¹³	1.4 Open questions	⁹
¹⁴	2 The JUNO experiment	¹¹
¹⁵	2.1 Neutrinos physics in JUNO	¹²
¹⁶	2.1.1 Reactor neutrino oscillation for NMO and precise measurements	¹²
¹⁷	2.1.2 Other physics	¹⁵
¹⁸	2.2 The JUNO detector	¹⁶
¹⁹	2.2.1 Detection principle	¹⁷
²⁰	2.2.2 Central Detector (CD)	¹⁸
²¹	2.2.3 Veto detector	²²
²²	2.3 Calibration strategy	²³
²³	2.3.1 Energy scale calibration	²³
²⁴	2.3.2 Calibration system	²⁴
²⁵	2.3.3 Instrumental non-linearity calibration	²⁴
²⁶	2.4 Satellite detectors	²⁵
²⁷	2.4.1 TAO	²⁵
²⁸	2.4.2 OSIRIS	²⁶
²⁹	2.5 Software	²⁷
³⁰	2.6 State of the art of the Offline IBD reconstruction in JUNO	²⁸
³¹	2.6.1 Interaction vertex reconstruction	²⁸
³²	2.6.2 Energy reconstruction	³²
³³	2.6.3 Machine learning for reconstruction	³⁴
³⁴	2.7 JUNO sensitivity to NMO and precise measurements	³⁷

35	2.7.1	Theoretical spectrum	37
36	2.7.2	Fitting procedure	38
37	2.7.3	Physics results	39
38	2.8	Summary	39
39	3	Machine learning and Artificial Neural Network	41
40	3.1	Boosted Decision Tree (BDT)	41
41	3.2	Artificial Neural Network (NN)	42
42	3.2.1	Fully Connected Deep Neural Network (FCDNN)	43
43	3.2.2	Convolutional Neural Network (CNN)	43
44	3.2.3	Graph Neural Network (GNN)	45
45	3.2.4	Adversarial Neural Network (ANN)	46
46	3.2.5	Training procedure	46
47	3.2.6	Potential pitfalls	49
48	4	Image recognition for IBD reconstruction with the SPMT system	53
49	4.1	Motivations	53
50	4.2	Method and model	54
51	4.2.1	Model	54
52	4.2.2	Data representation	56
53	4.2.3	Dataset	57
54	4.2.4	Data characteristics	58
55	4.3	Training	60
56	4.4	Results	61
57	4.4.1	J21 results	62
58	4.4.2	J21 Combination of classic and ML estimator	63
59	4.4.3	J23 results	66
60	4.5	Conclusion and prospect	67
61	5	Graph representation of JUNO for IBD reconstruction	69
62	5.1	Motivation	69
63	5.2	Data representation	70
64	5.3	Message passing algorithm	72
65	5.4	Data	74
66	5.5	Model	75
67	5.6	Training	76
68	5.7	Optimization	76
69	5.8	Results	77
70	5.9	Conclusion	78
71	6	Reliability of machine learning methods	81
72	7	Joint fit between the SPMT and LPMT spectra	83
73	7.1	Motivations	84

74	7.1.1	Discrepancies between the SPMT and LPMT results	84
75	7.1.2	Charge Non-Linearity (QNL)	84
76	7.2	Approach	85
77	7.2.1	Data production	85
78	7.2.2	Individual fits	87
79	7.3	Fit framework	87
80	7.3.1	IBD generator	87
81	7.4	Technical challenges	87
82	7.5	Results	87
83	7.5.1	Covariance matrix	87
84	7.6	Conclusion and perspectives	87
85	8	Conclusion	89
86	A	Calculation of optimal α for estimator combination	91
87	A.1	Unbiased estimator	91
88	A.2	Optimal variance estimator	91
89	B	Charge spherical harmonics analysis	93
90	List of Tables		101
91	List of Figures		108
92	List of Abbreviations		109
93	Bibliography		111

Remerciements

94

95 Introduction

⁹⁶ **Chapter 1**

⁹⁷ **Neutrino physics**

⁹⁸

The neutrino, or ν for the close friends, a fascinating and invisible particle. Some will say that dark matter also have those property but at least we are pretty confident that neutrinos exists.

⁹⁹ **1.1 Standard model**

¹⁰⁰ **1.1.1 Limits of the standard model**

¹⁰¹ **1.2 Historic of the neutrino**

¹⁰² **First theories**

¹⁰³ **Discovery**

¹⁰⁴ **Milestones and anomalies**

¹⁰⁵ **1.3 Oscillation**

¹⁰⁶ **1.3.1 Phenomologies**

¹⁰⁷ **1.4 Open questions**

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¹⁰⁸ **Chapter 2**

¹⁰⁹ **The JUNO experiment**

¹¹⁰ "Ave Juno, rosae rosam, et spiritus rex". It means nothing but I found it in tone.

¹¹¹ The first idea of a medium baseline (~ 52 km) experiment, was explored in 2008 [1] where it was
¹¹² demonstrated that the Neutrino Mass Ordering (NMO) could be determined by a medium baseline
¹¹³ experiment if $\sin^2(2\theta_{13}) > 0.005$ without the requirements of accurate knowledge of the reactor
¹¹⁴ antineutrino spectra and the value of Δm_{32}^2 . From this idea is born the Jiangmen Underground
¹¹⁵ Neutrino Observatory (JUNO) experiment.

¹¹⁶ JUNO is a neutrino detection experiment under construction located in China, in Guangdong prov-
¹¹⁷ ing, near the city of Kaiping. Its main objectives are the determination of the mass ordering at the
¹¹⁸ $3\text{-}4\sigma$ level in 6 years of data taking and the measurement at the sub-percent precision of the oscillation
¹¹⁹ parameters Δm_{21}^2 , $\sin^2 \theta_{12}$, Δm_{32}^2 and with less precision $\sin^2 \theta_{13}$ [2].



FIGURE 2.1 – On the left: Location of the JUNO experiment and its reactor sources in southern China. On the right: Aerial view of the experimental site

¹²⁰ For this JUNO will measure the electronic anti-neutrinos ($\bar{\nu}_e$) flux coming from the nuclear reactors
¹²¹ of Taishan, Yangjiang, for a total power of 26.6 GW_{th} , and the Daya Bay power plant to a lesser
¹²² extent. All of those cores are the second-generation pressurized water reactors CPR1000, which is a
¹²³ derivative of Framatome M310. Details about the power plants characteristics and their expected flux
¹²⁴ of $\bar{\nu}_e$ can be found in the table 2.1. The distance of 53 km has been specifically chosen to maximize
¹²⁵ the disappearance probability of the $\bar{\nu}_e$. The data taking is scheduled to start early 2025.

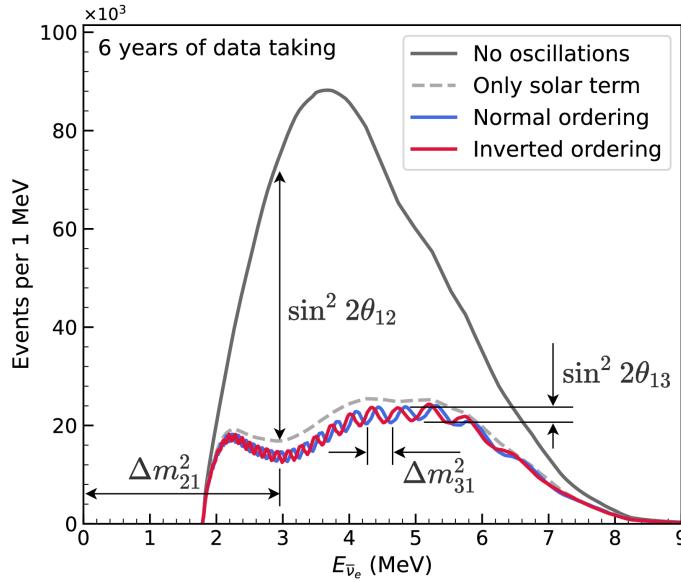


FIGURE 2.2 – Expected number of neutrinos event per MeV in JUNO after 6 years of data taking. The black curve shows the flux if there was no oscillation. The light gray curve shows the oscillation if only the solar terms are taken in account (θ_{12} , Δm_{21}^2). The blue and red curve shows the spectrum in the case of, respectively, NO and IO. The dependency of the oscillation to the different parameters are schematized by the double sided arrows. We can see the NMO sensitivity by looking at the fine phase shift between the red and the blue curve.

¹²⁶ 2.1 Neutrinos physics in JUNO

¹²⁷ Even if the JUNO design detailed in section 2.2 was optimized for the measurement of the NMO, its
¹²⁸ large detection volume, excellent energy resolution and background level and understanding make it
¹²⁹ also an excellent detector to measure the flux coming from other neutrino sources. Thus the scientific
¹³⁰ program of JUNO extends way over reactor antineutrinos. The following section is an overview of
¹³¹ the different physics topic JUNO will contribute in the coming years.

¹³² 2.1.1 Reactor neutrino oscillation for NMO and precise measurements

Previous works [1, 3] shows that oscillation parameters and the NMO can be observed by looking at the $\bar{\nu}_e$ disappearance energy spectrum coming from medium baseline nuclear reactor. This disappearance probability can be expressed as [2] :

$$P(\bar{\nu}_e \rightarrow \bar{\nu}_e) = 1 - \sin^2 2\theta_{12} c_{13}^4 \sin^2 \frac{\Delta m_{21}^2 L}{4E} - \sin^2 2\theta_{13} \left[c_{12}^2 \sin^2 \frac{\Delta m_{31}^2 L}{4E} + s_{12}^2 \sin^2 \frac{\Delta m_{32}^2 L}{4E} \right]$$

¹³³ Where $s_{ij} = \sin \theta_{ij}$, $c_{ij} = \cos \theta_{ij}$, E is the $\bar{\nu}_e$ energy and L is the baseline. We can see the sensitivity
¹³⁴ to the NMO in the dependency to Δm_{32}^2 and Δm_{31}^2 causing a phase shift of the spectrum as we can
¹³⁵ see in the figure 2.2. By carefully adjusting a theoretical spectrum to the data, one can extract the
¹³⁶ NMO and the oscillation parameters. The statistic procedure used to adjust the theoretical spectrum
¹³⁷ is reviewed in more details in the section 2.7. To reach the desired sensitivity, JUNO must meet
¹³⁸ multiple requirements but most notably:

- 139 1. An energy resolution of $3\%/\sqrt{E(\text{MeV})}$ to be able to distinguish the fine structure of the fast
140 oscillation.
- 141 2. An energy precision of 1% in order to not err on the location of the oscillation pattern.
- 142 3. A baseline between 40 and 65 km to maximise the $\bar{\nu}_e$ oscillation probability. The optimal
143 baseline would be 58 km and JUNO baseline is 53 km.
- 144 4. At least $\approx 100,000$ events to limit the spectrum distortion due to statistical uncertainties.

145 $\bar{\nu}_e$ flux coming from nuclear power plants

146 To get such high measurements precision, it is necessary to have a very good understanding of the
147 sources characteristics. For its NMO and precise measurement studies, JUNO will observe the energy
148 spectrum of neutrinos coming from the nuclear power plants Taishan and Yangjiang's cores, located
149 at 53 km of the detector to maximise the disappearance probability of the $\bar{\nu}_e$.

Reactor	Power (GW _{th})	Baseline (km)	IBD Rate (day ⁻¹)	Relative Flux (%)
Taishan	9.2	52.71	15.1	32.1
Core 1	4.6	52.77	7.5	16.0
Core 2	4.6	52.64	7.6	16.1
Yangjiang	17.4	52.46	29.0	61.5
Core 1	2.9	52.74	4.8	10.1
Core 2	2.9	52.82	4.7	10.1
Core 3	2.9	52.41	4.8	10.3
Core 4	2.9	52.49	4.8	10.2
Core 5	2.9	52.11	4.9	10.4
Core 6	2.9	52.19	4.9	10.4
Daya Bay	17.4	215	3.0	6.4

TABLE 2.1 – Characteristics of the nuclear power plants observed by JUNO. The IBD rate are estimated from the baselines, the reactors full thermal power, selection efficiency and the current knowledge of the oscillation parameters

150 The $\bar{\nu}_e$ coming from reactors are emitted from β -decay of unstable fission fragments. The Taishan
151 and Yangjiang reactors are Pressurised Water Reactor (PWR), the same type as Daya Bay. In those
152 type of reactor more the 99.7 % and $\bar{\nu}_e$ are produced by the fissions of four fuel isotopes ^{235}U , ^{238}U ,
153 ^{239}Pu and ^{241}Pu . The neutrino flux per fission of each isotope is determined by the inversion of the
154 measured β spectra of fission product [4–8] or by calculation using the nuclear databases [9, 10].

155 The neutrino flux coming from a reactor at a time t can be predicted using

$$\phi(E_\nu, t)_r = \frac{W_{th}(t)}{\sum_i f_i(t) e_i} \sum_i f_i(t) S_i(E_\nu) \quad (2.1)$$

156 where $W_{th}(t)$ is the thermal power of the reactor, $f_i(t)$ is the fraction fission of the i th isotope, e_i its
157 thermal energy released in each fission and $S_i(e_\nu)$ the neutrino flux per fission for this isotope. Using
158 this method, the flux uncertainty is expected to be of an order of 2-3 % [11].

159 In addition to those prediction, a satellite experiment named TAO[12] will be setup near the reactor
160 core Taishan-1 to measure with an energy resolution of 2% at 1 MeV the neutrino flux coming from
161 the core, more details can be found in section 2.4.1. It will help identifying unknown fine structure
162 and give more insight on the $\bar{\nu}_e$ flux coming from this reactor.

163 One the open issue about reactor anti-neutrinos flux is the so-called neutrino anomaly [13], an
164 unexpected surplus of neutrino emission in the spectra around 5 MeV. Multiples scientists are trying

165 to explain this surplus by advanced recalculation of the nuclei model during beta decay [14, 15] but
 166 no consensus on this issue has been reached yet.

167 **Background in the neutrinos reactor spectrum**

168 Considering the close reactor neutrinos flux as the main signal, the signals that are considered as
 169 background are:

- 170 — The geoneutrinos producing background in the $0.511 \sim 2.7$ MeV region.
- 171 — The neutrinos coming from the other nuclear reactors around Earth.

172 In addition to all those physics signal, non-neutrinos signal that would mimic an IBD will also be
 173 present. It is composed of:

- 174 — The signal coming from radioactive decay (α , γ , β) from natural radioactive isotopes in the
 material of the detector.
- 175 — Cosmogenic event such as fast neutrons and activated isotopes induced by muons passing
 177 through the detector, most notably the spallation on ^{12}C .

178 All those events represent a non-negligable part of the spectrum as shown in figure 2.3.

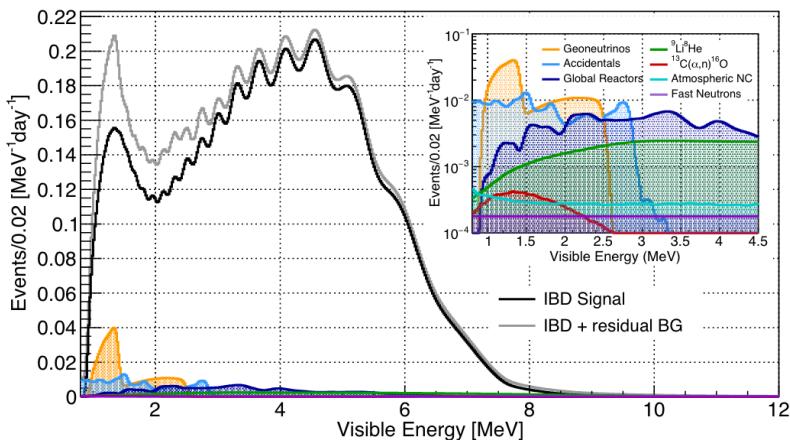


FIGURE 2.3 – Expected visible energy spectrum measured with the LPMT system with (grey) and without (black) backgrounds. The background amount for about 7% of the IBD candidate and are mostly localized below 3 MeV [11]

179 **Identification of the mass ordering**

180 To identify the mass ordering, we adjust the theoretical neutrino energy spectrum under the two
 181 hypothesis of NO and IO. Those give us two χ^2 , respectively χ^2_{NO} and χ^2_{IO} . By computing the
 182 difference $\Delta\chi^2 = \chi^2_{NO} - \chi^2_{IO}$ we can determine the most probable mass ordering and the confidence
 183 interval: NO if $\Delta\chi^2 > 0$ and IO if $\Delta\chi^2 < 0$. Current studies shows that the expected sensitivity
 184 the mass ordering would be of 3.4σ after 6 years of data taking in nominal setup[2]. More detailed
 185 explanations about the procedure can be found in the section 2.7.

186 **Precise measurement of the oscillations parameters**

187 The oscillations parameters θ_{12} , θ_{13} , Δm_{21}^2 , Δm_{31}^2 are free parameters in the fit of the oscillation
 188 spectrum. The precision on those parameters have been estimated and are shown in table 2.2. Wee
 189 see that for θ_{12} , Δm_{21}^2 , Δm_{31}^2 , precision at 6 years is better than the reference precision by an order of
 190 magnitude [11]

	Central Value	PDG 2020	100 days	6 years	20 years
$\Delta m_{31}^2 (\times 10^{-3} \text{ eV}^2)$	2.5283	± 0.034 (1.3%)	± 0.021 (0.8%)	± 0.0047 (0.2%)	± 0.0029 (0.1%)
$\Delta m_{21}^2 (\times 10^{-3} \text{ eV}^2)$	7.53	± 0.18 (2.4%)	± 0.074 (1.0%)	± 0.024 (0.3%)	± 0.017 (0.2%)
$\sin^2 \theta_{12}$	0.307	± 0.013 (4.2%)	± 0.0058 (1.9%)	± 0.0016 (0.5%)	± 0.0010 (0.3%)
$\sin^2 \theta_{13}$	0.0218	± 0.0007 (3.2%)	± 0.010 (47.9%)	± 0.0026 (12.1%)	± 0.0016 (7.3%)

TABLE 2.2 – A summary of precision levels for the oscillation parameters. The reference value (PDG 2020 [16]) is compared with 100 days, 6 years and 20 years of JUNO data taking.

2.1.2 Other physics

While the design of JUNO is tailored to measure $\bar{\nu}_e$ coming from nuclear reactor, JUNO will be able to detect neutrinos coming from other sources thus allowing for a wide range of physics studies as detailed in the table 2.3 and in the following sub-sections.

Research	Expected signal	Energy region	Major backgrounds
Reactor antineutrino	60 IBDs/day	0–12 MeV	Radioactivity, cosmic muon
Supernova burst	5000 IBDs at 10 kpc	0–80 MeV	Negligible
DSNB (w/o PSD)	2300 elastic scattering		
Solar neutrino	2–4 IBDs/year	10–40 MeV	Atmospheric ν
Atmospheric neutrino	hundreds per year for ${}^8\text{B}$	0–16 MeV	Radioactivity
Geoneutrino	hundreds per year	0.1–100 GeV	Negligible
	≈ 400 per year	0–3 MeV	Reactor ν

TABLE 2.3 – Detectable neutrino signal in JUNO and the expected signal rates and major background sources

Geoneutrinos

Geoneutrinos designate the antineutrinos coming from the decay of long-lived radioactive elements inside the Earth. The 1.8 MeV threshold necessary for the IBD makes it possible to measure geoneutrinos from ${}^{238}\text{U}$ and ${}^{232}\text{Th}$ decay chains. The studies of geoneutrinos can help refine the Earth crust models but is also necessary to characterise their signal, as they are a background to the mass ordering and oscillations parameters studies.

Atmospheric neutrinos

Atmospheric neutrinos are neutrinos originating from the decay of π and K particles that are produced in extensive air showers initiated by the interactions of cosmic rays with the Earth atmosphere. Earth is mostly transparent to neutrinos below the PeV energy, thus JUNO will be able to see neutrinos coming from all directions. Their baseline range is large (15km \sim 13000km), they can have energy between 0.1 GeV and 10 TeV and will contain all neutrino and antineutrinos flavour. Their studies is complementary to the reactor antineutrinos and can help refine the constraints on the NMO [2].

Supernovae burst neutrinos

Neutrinos are crucial component during all stages of stellar collapse and explosion. Detection of neutrinos coming for core collapse supernovae will provide us important informations on the mech-

212 mechanisms at play in those events. Thanks to its 20 kt sensible volume, JUNO has excellent capabilities
 213 to detect all flavour of the $\mathcal{O}(10 \text{ MeV})$ postshock neutrinos, and using neutrinos of the $\mathcal{O}(1 \text{ MeV})$
 214 will give informations about the pre-supernovae neutrinos. All those informations will allow to
 215 disentangle between the multiple hydro-dynamic models that are currently used to describe the
 216 different stage of core-collapse supernovae.

217 Diffuse supernovae neutrinos background

218 Core-collapse supernovae in our galaxy are rare events, but they frequently occur throughout the
 219 visible Universe sending burst of neutrinos in direction of the Earth. All those events contributes to
 220 a low background flux of low-energy neutrinos called the Diffuse Supernovae Neutrino Background
 221 (DSNB). Its flux and spectrum contains informations about the red-shift dependent supernovae rate,
 222 the average supernovae neutrino energy and the fraction of black-hole formation in core-collapse su-
 223 pernovae. Depending of the DSNB model, we can expect 2-4 IBD events per year in the energy range
 224 above the reactor $\bar{\nu}_e$ signal, which is competitive with the current Super-Kamiokande+Gadolinium
 225 phase [17].

226 Beyond standard model neutrinos interactions

227 JUNO will also be able to probe for beyond standard model neutrinos interactions. After the main
 228 physics topics have been accomplished, JUNO could be upgraded to probe for neutrinoless beta
 229 decay ($0\nu\beta\beta$). The detection of such event would give critical informations about the nature of
 230 neutrinos, is it a majorana or a dirac particle. JUNO will also be able to probe for neutrinos that
 231 would come for the decay or annihilation of Dark Matter inside the sun and neutrinos from putative
 232 primordial black hole. Through the unitary test of the mixing matrix, JUNO will be able to search for
 233 light sterile neutrinos. Thanks to JUNO sensitivity, multiple other exotic research can be performed
 234 on neutrino related beyond standard model interactions.

235 Proton decay

236 Proton decay is a potential unobserved event where the proton decay by violating the baryon num-
 237 ber. This violation is necessary to explain the baryon asymmetry in the universe and is predicted
 238 by multiple Grand Unified Theories which unify the strong, weak and electromagnetic interactions.
 239 Thanks to its large active volume, JUNO will be able to take measurement of the potential proton
 240 decay channel $p \rightarrow \bar{\nu}K^+$. Study [18] show that JUNO should be competitive with the current best
 241 limit at 5.9×10^{33} years from Super-K. This studies show that JUNO, considering no proton decay
 242 events observed, would be able to rules a limit of 9.6×10^{33} years at 90 % C.L.

243 2.2 The JUNO detector

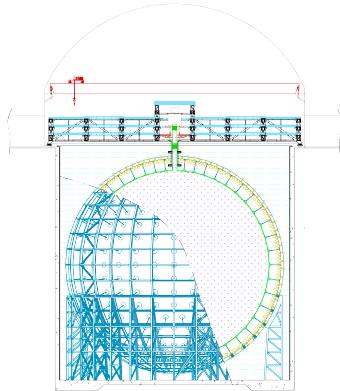
244 The JUNO detector is a scintillator detector buried 693.35 meters under the ground (1800 meters
 245 water equivalent). It consist of Central Detector (CD), a water pool and a Top Tracker (TT) as showed
 246 in figure 2.4a. The CD is an acrylic vessel containing the 20 ktons of Liquid Scintillator (LS). It is
 247 supported by a stainless steel structure and is immersed in that water pool that is used as shielding
 248 from external radiation and as a cherenkov detector for the background. The top of the experiment
 249 is partially covered by the Top Tracker (TT), a plastic scintillator detector which is use to detect the
 250 atmospheric muons background and is acting as a veto detector.

251 The top of the experiment also host the LS purification system, a water purification system, a ven-
 252 tilation system to get rid of the potential radon in the air. The CD is observed by two system of

253 Photo-Multipliers Tubes (PMT). They are attached to the steel structure and their electronic readout
 254 is submersed near them. A third system of PMT is also installed on the structure but are facing
 255 outward of the CD, instrumenting the water to be cherenkov detector. The CD and the cherenkov
 256 detector are optically separated by Tyvek sheet. A chimney for LS filling and purification and for
 257 calibration operations connects the CD to the experimental hall from the top.

258 The CD has been dimensioned to meet the requirements presented in section 2.1.1:

- 259 — Its 20 ktons monolithic LS provide a volume sizeable enough, in combination with the ex-
 260 pected $\bar{\nu}_e$ flux, to reach the desired statistic in 6 years. Its monolithic nature also allow for a
 261 full containment of most of the events, preventing the energy loss in non-instrumented parts
 262 that would arise from a segmented detector.
- 263 — Its large overburden shield it from most of the atmospheric background that would pollute
 264 the signal.
- 265 — The localization of the experiment, chosen to maximize the disappearance with a 53km base-
 266 line and in a region that allow two nuclear power plant to be used as sources.



(A) Schematics view of the JUNO detector.



(B) Top down view of the JUNO detector under construction

FIGURE 2.4

267 This section cover in details the different components of the detector and the detection systems.

268 2.2.1 Detection principle

The CD will detect the neutrino and measure their energy mainly via an Inverse Beta Decay (IBD) interaction with proton mainly from the ^{12}C and H nucleus in the LS:

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

269 Kinematics calculation shows that this interaction has an energy threshold for the $\bar{\nu}_e$ of $(m_n + m_e -$
 270 $m_p) \approx 1.806$ MeV [19]. This threshold make the experiment blind to very low energy neutrinos.
 271 The residual energy $E_\nu - 1.806$ MeV is be distributed as kinetic energy between the positron and the
 272 neutron. The energy of the emitted positron E_e is given by [19]

$$E_e = \frac{(E_\nu - \delta)(1 + \epsilon_\nu) + \epsilon_\nu \cos \theta \sqrt{(E_\nu - \delta)^2 + \kappa m_e^2}}{\kappa} \quad (2.2)$$

273 where $\kappa = (1 + \epsilon_\nu)^2 - \epsilon_\nu^2 \cos^2 \theta \approx 1$, $\epsilon_\nu = \frac{E_\nu}{m_p} \ll 1$ and $\delta = \frac{m_n^2 - m_p^2 - m_e^2}{2m_p} \ll 1$. We can see from this
 274 equation that the positron energy is strongly correlated to the neutrino energy.

The positron and the neutron will then propagate in the detection medium, the Liquid Scintillator (LS), loosing their kinetic energy by exciting the molecule of the LS (more details in section 2.2.2). Once stopped, the positron will annihilate with an electron from the medium producing two 511 KeV gamma. Those gamma will themselves interact with the LS, exciting it before being absorbed by photoelectrical effect. The neutron will be captured by an hydrogen, emitting a 2.2 MeV gamma in the process. This gamma will also deposit its energy before being absorbed by the LS.

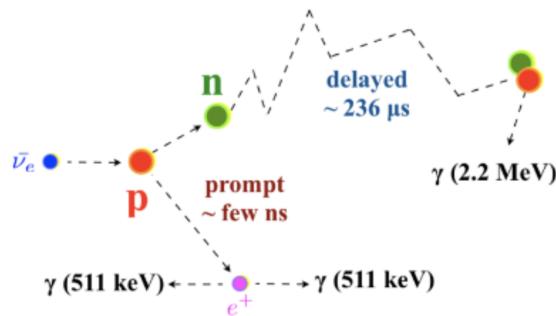


FIGURE 2.5 – Schematics of an IBD interaction in the central detector of JUNO

The scintillation photons have frequency in the UV and will propagate in the LS, being re-absorbed and re-emitted by compton effect before finally be captured by PMTs instrumenting the acrylic sphere. The analog signal of the PMTs digitized by the electronic is the signal of our experiment. The signal produced by the positron is subsequently called the prompt signal, and the signal coming from the neutron the delayed signal. This naming convention come from the fact that the positron will deposit its energy rather quickly (few ns) where the neutron will take a bit more time ($\sim 236 \mu\text{s}$).

2.2.2 Central Detector (CD)

The central detector, composed of 20 ktons of Liquid Scintillator (LS), is the main part of JUNO. The LS is contained in a spherical acrylic vessel supported by a stainless steel structure. The CD and its structural support are submerged in a cylindrical water pool of 43.5m diameter and 44m height. We're confident that the water pool provide sufficient buffer protection in every direction against the rock radioactivity.

Acrylic vessel

The acrylic vessel is a spherical vessel of inner diameter of 35.4 m and a thickness of 120 mm. It is assembled from 265 acrylic panels, thermo bonded together. The acrylic recipes has been carefully tuned with extensive R&D to ensure it does not include plasticizer and anti-UV material that would stop the scintillation photons. Those panels requires to be pure of radioactive materials to not cause background. Current setup where the acrylic panels are molded in cleanrooms of class 10000, let us reach a uranium and thorium contamination of <0.5 ppt. The molding and thermoforming processes is optimized to increase the assemblage transparency in water to >96%. The acrylic vessel is supported by a stainless steel structure via supporting node (fig 2.6). The structure and the nodes are designed to be resilient to natural catastrophic events such as earthquake and can support many times the effective load of the acrylic vessel.

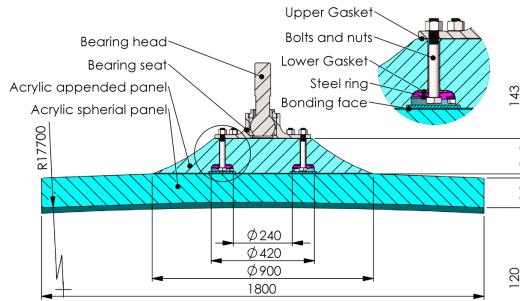


FIGURE 2.6 – Schematics of the supporting node for the acrylic vessel

304 **Liquid scintillator**

305 The Liquid Scintillator (LS) has a similar recipe as the one used in Daya Bay [20] but without gadolinium
 306 doping. It is made of three components, necessary to shift the wavelength of emitted photons to
 307 prevent their reabsorption and to shift their wavelength to the PMT sensitivity region as illustrated
 308 in figure 2.7:

- 309 1. The detection medium, the *linear alkylbenzene* (LAB). Selected because of its excellent trans-
 310 parency, high flash point, low chemical reactivity and good light yield. Accounting for \sim
 311 98% of the LS, it is the main component with which ionizing particles and gamma interact.
 312 Charged particles will collide with its electronic cloud transferring energy to the molecules,
 313 gamma will interact via compton effect with the electronic cloud before finally be absorbed
 314 via photoelectric effect.
- 315 2. The second component of the LS is the *2,5-diphenyloxazole* (PPO). A fraction of the excitation
 316 energy of the LAB is transferred to the PPO, mainly via non radiative process [21]. The
 317 PPO molecules de-excites in the same way, transferring their energy to the bis-MSB. The PPO
 318 makes for 1.5 % of the LS.
- 319 3. The last component is the *p-bis(o-methylstyryl)-benzene* (bis-MSB). Once excited by the PPO, it
 320 will emit photon with an average wavelength of \sim 430 nm (full spectrum in figure 2.7) that
 321 can thus be detected by our photo-multipliers systems. It amount for \sim 0.5% of the LS.

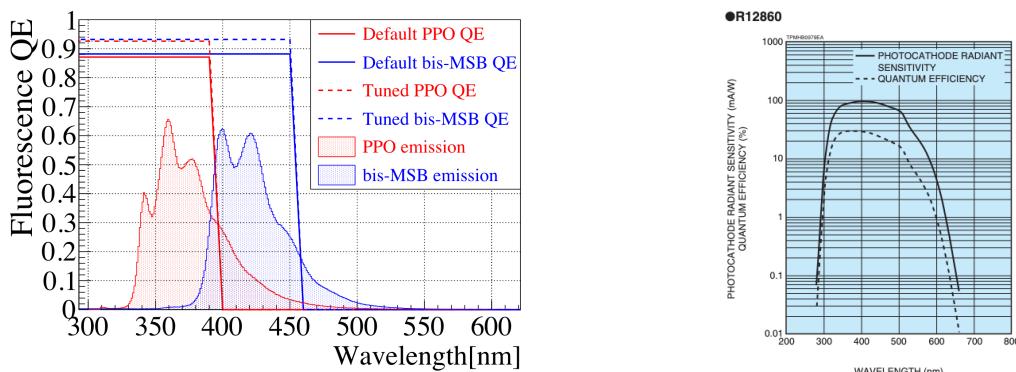


FIGURE 2.7 – On the left: Quantum efficiency (QE) and emission spectrum of the LAB and the bis-MSB [20]. On the right: Sensitivity of the Hamamatsu LPMT depending on the wavelength of the incident photons [22].

322 This formula has been optimized using dedicated studies with a Daya Bay detector [20, 23] to reach
 323 the requirements for the JUNO experiment:

- 324 — A light yield / MeV of the amount of 10^4 photons to maximize the statistic in the energy
 325 measurement.

- An attenuation length comparable to the size of the detector to prevent losing photons during their propagation in the LS. The final attenuation length is 25.8m [24] to compare with the CD diameter of 35.4m.
- Uranium/Thorium radiopurity to prevent background signal. The reactor neutrino program require a contamination fraction $F < 10^{-15}$ while the solar neutrino program require $F < 10^{-17}$.

The LS will frequently be purified and tested in the Online Scintillator Internal Radioactivity Investigation System (OSIRIS) [25] to ensure that the requirements are kept during the lifetime of the experiment, more details to be found in section 2.4.2.

335 Large Photo-Multipliers Tubes (LPMTs)

336 The scintillation light produced by the LS is then collected by Photo-Multipliers Tubes (PMT) that
 337 transform the incoming photon into an electric signal. As described in figure 2.8, the incident photons
 338 interact with the photocathode via photoelectric effect producing an electron called a Photo-Electron
 339 (PE). This PE is then focused on the dynodes where the high voltage will allow it to be multiplied.
 340 After multiple amplification the resulting charge - in coulomb [C] - is collected by the anode and
 341 the resulting electric signal can be digitalized by the readout electronics from which the charge and
 342 timing can be extracted.

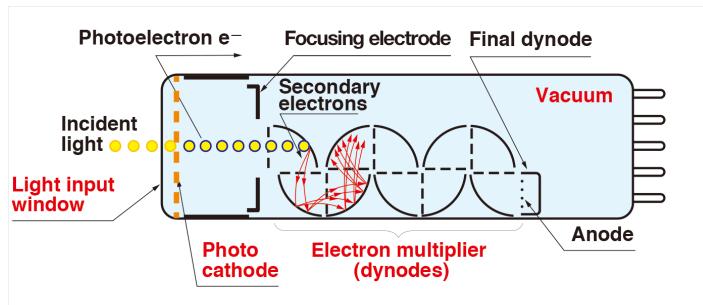


FIGURE 2.8 – Schematic of a PMT

343 The Large Photo-Multipliers Tubes (LPMT), used in the central detector and in the water pool, are
 344 20-inch (50.8 cm) radius PMTs. ~ 5000 dynode-PMTs [22] were produced by the Hamamatsu[®]
 345 company and ~ 15000 Micro-Channel Plate (MCP) [26] by the NNVT[®] company. This system is
 346 the one responsible for the energy measurement with a energy resolution of $3\%/\sqrt{E}$, resolution
 347 necessary for the mass ordering measurement. To reach this precision, the system is composed of
 348 17612 PMTs quasi uniformly distributed over the detector for a coverage of 75.2% reaching ~ 1800
 349 PE/MeV or $\sim 2.3\%$ resolution due to statistic, leaving $\sim 0.7\%$ for the systematic uncertainties. They
 350 are located outside the acrylic sphere in the water pool facing the center of the detector. To maintain
 351 the resolution over the lifetime of the experiment, JUNO require a failure rate $< 1\%$ over 6 years.

352 The LPMTs electronic are divided in two parts. One "near", located underwater, in proximity of the
 353 LPMT to reduce the cable length between the PMT and early electronic. A second one, outside of the
 354 detector that is responsible for higher level analysis before sending the data to the DAQ.

355 The light yield per MeV induce that a LPMT can collect between 1 and 1000 PE per event, a wide
 356 dynamic range, causing non linearity in the PMT response that need to be understood and calibrated,
 357 see section 2.3 for more details.

358 Before performing analysis, the analog readout of the LPMT need to be amplified, digitised and
 359 packaged by the readout electronics schematized in figure 2.9. This electronic is splitted in two parts:
 360 *wet* electronic that are located near the LPMTs, protected in an Underwater Box (UWB) and the *dry*
 361 electronics located in deicated rooms outside of the water pool.

The LPMTs are connected to the UWB by groups of three. Each UWB contains:

- Three high voltage units, each one powering a PMT.
- A global control unit, responsible for the digitization of the waveform, composed of six analog-digital units that produce digitized waveform and a Field Programmable Gate Array (FPGA) that complete the waveform with metadatas such as the local timestamp trigger, etc... This FPGA also act as a data buffer when needed by the DAQ and trigger system.
- Additional memory in order to temporally store the data in case of sudden burst of the input rate (such as in the case of nearby supernovae).

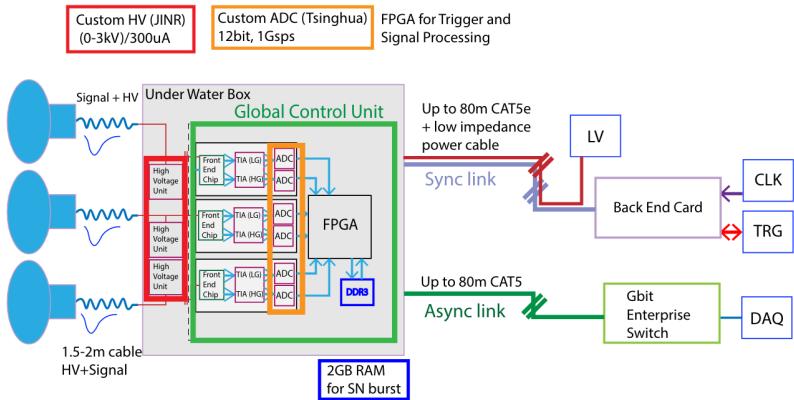


FIGURE 2.9 – The LPMT electronics scheme. It is composed of two part, the *wet* electronics on the left, located underwater and the *dry* electronics on the right. They are connected by Ethernet cable for data transmission and a dedicated low impedance cable for power distribution

The *dry* electronic synchronize the signals from the UWBs and centralise the information of the CD LPMTs. It act as the Global Trigger by sending the UWB data to DAQ in the case if the LPMT multiplicity condition is fulfilled.

Small Photo-Multipliers Tubes (SPMTs)

The Small PMT (SPMTs) system is made of 3-inch (7.62 cm) PMTs. They will be used in the CD as a secondary detection system. Those 25600 SPMTs will observe the same events as the LPMTs, thus sharing the physics and detector systematics up until the photon conversion. With a detector coverage of 2.7%, this system will collect ~ 43 PE/MeV for a final energy resolution of $\sim 17\%$. This resolution is not enough to measure the NMO, θ_{13} , Δm^2_{31} but will be sufficient to independently measure θ_{12} and Δm^2_{21} .

The benefit of this second system is to be able to perform another, independent measure of the same events as the LPMTs, constituting the Dual Calorimetry. Due to the low PE rate, SPMTs will be running in photo-counting mode in the reactor range and thus will be insensitive to non-linearity effect. Using this property, the intrinsic charge non linearity of the LPMTs can be measured by comparing the PE count in the SPMTs and LPMTs [27]. Also, due to their smaller size and electronics, SPMTs have a better timing resolutions than the LPMTs. At higher energy range, like supernovae events, LPMTs will saturate where SPMTs due to their lower PE collection will produce a reliable measure of the energy spectrum.

The SPMTs will be grouped by pack of 128 to an UWB hosting their electronics as illustrated in figure 2.10. This underwater box host two high voltage splitter boards, each one supplying 64 SPMTs, an ASIC Battery Card (ABC) and a global control unit.

391 The ABC board will readout and digitize the charge and time of the 128 SPMTs signals and a FPGA
 392 will joint the different metadata. The global control unit will handle the powering and control of the
 393 board and will be in charge of the transmission of the data to the DAQ.

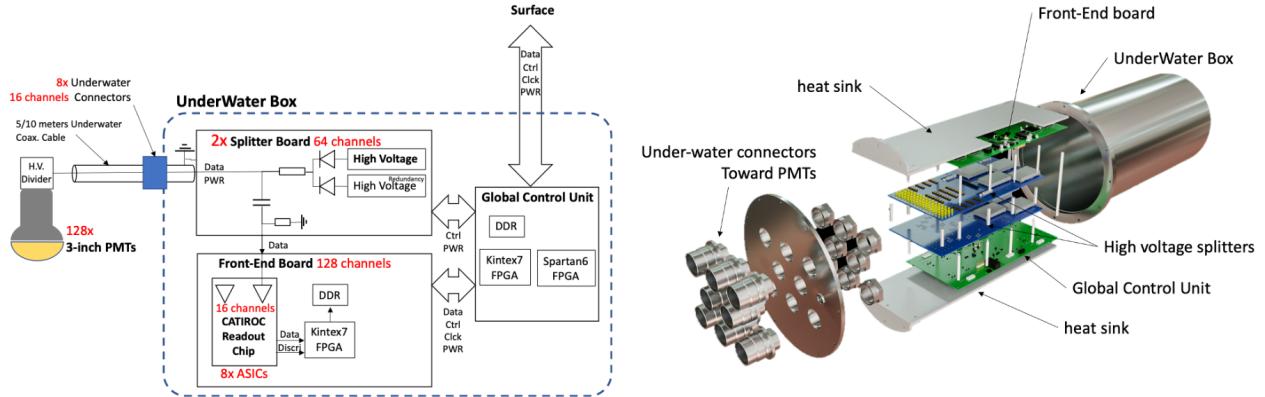


FIGURE 2.10 – Schematic of the JUNO SPMT electronic system (left), and exploded view of the main component of the UWB (right)

394 2.2.3 Veto detector

395 The CD will be bathed in constant background noise coming from numerous sources : the radioac-
 396 tivity from surrounding rock and its own components or from the flux of cosmic muons. This
 397 background needs to be rejected to ensure the purity of the IBD spectrum. To prevent a big part
 398 of them, JUNO use two veto detector that will tag events as background before CD analysis.

399 Cherenkov in water pool

400 The Water Cherenkov Detector (WCD) is the instrumentation of the water buffer around the CD.
 401 When high speed charged particles will pass through the water, they will produce cherenkov
 402 photons. The light will be collected by 2400 MCP LPMTs installed on the outer surface of the CD
 403 structure. The muons veto strategy is based on a PMT multiplicity condition. WCD PMTs are
 404 grouped in ten zones: 5 in the top, 5 in the bottom. A veto is raised either when more than 19
 405 PMTs are triggered in one zone or when two adjacent zones simultaneously trigger more than 13
 406 PMTs. Using this trigger, we expect to reach a muon detection efficiency of 99.5% while keeping the
 407 noise at reasonable level.

408 Top tracker

409 The JUNO Top Tracker (TT) is a plastic scintillator detector located on the top of the experiment (see
 410 figure 2.11). Made from plastic scintillator from OPERA [28] layered horizontally in 3 layers on the
 411 top of the detector, the TT will be able to detect incoming atmospheric muons. With its coverage,
 412 about 1/3 of the of all atmospheric muons that passing through the CD will also pass through the 3
 413 layer of the detector. While it does not cover the majority of the CD, the TT is particularly effective
 414 to detect muons coming through the filling chimney region which might present difficulties from the
 415 other subsystems in some classes of events.

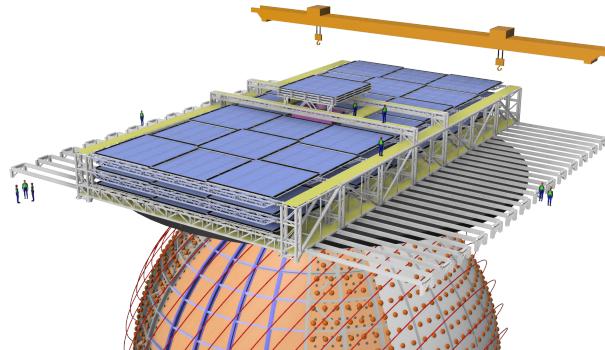


FIGURE 2.11 – The JUNO top tracker

416 2.3 Calibration strategy

417 The calibration is a crucial part of the JUNO experiment. The detector will continuously bath in
 418 neutrinos coming from the close nuclear power plant, from other sources such as geo neutrinos,
 419 the sun and will be exposed to background noise coming from atmospheric muons and natural
 420 radioactivity. Because of this continuous rate, low frequency signal event, we need high frequency,
 421 recognisable sources in the energy range of interest : [0-12] MeV for the positron signal and 2.2 MeV
 422 for the neutron capture. It is expected that the CD response will be different depending on the type
 423 of particle, due to the interaction with LS, the position on the event and the optical response of the
 424 acrylic sphere (see section 2.6). We also expect a non-linear energy response of the CD due to the LS
 425 properties [20] but also due to the saturation of the LPMTs system when collecting a large amount of
 426 PE [27].

427 2.3.1 Energy scale calibration

428 While electrons and positrons sources would be ideal, for a large LS detector thin-walled electrons
 429 or positrons sources could lead to leakage of radionucleides causing radioactive contamination.
 430 Instead, we consider gamma sources in the range of the prompt energy of IBDs. The sources are
 431 reported in table 2.4.

Sources / Processes	Type	Radiation
^{137}Cs	γ	0.0662 MeV
^{54}Mn	γ	0.835 MeV
^{60}Co	γ	1.173 + 1.333 MeV
^{40}K	γ	1.461 MeV
^{68}Ge	e^+	annihilation 0.511 + 0.511 MeV
$^{241}\text{Am-Be}$	n, γ	neutron + 4.43 MeV ($^{12}\text{C}^*$)
$^{241}\text{Am-}^{13}\text{C}$	n, γ	neutron + 6.13 MeV ($^{16}\text{O}^*$)
$(n, \gamma)p$	γ	2.22 MeV
$(n, \gamma)^{12}\text{C}$	γ	4.94 MeV or 3.68 + 1.26 MeV

TABLE 2.4 – List of sources and their process considered for the energy scale calibration

432 For the ^{68}Ge source, it will decay in ^{68}Ga via electron capture, which will itself β^+ decay into ^{68}Zn .
 433 The positrons will be absorbed by the enclosure so only the annihilation gamma will be released. In
 434 addition, (α, n) sources like $^{241}\text{Am-Be}$ and $^{241}\text{Am-}^{13}\text{C}$ are used to provide both high energy gamma
 435 and neutrons, which will later be captured in the LS producing the 2.2 MeV gamma.

From this calibration we call E_{vis} the "visible energy" that is reconstructed by our current algorithms and we compare it to the true energy deposited by the calibration source. The results shown in figure 2.12 show the expected response of the detector from calibration sources. The non-linearity is clearly visible from the E_{vis} / E_{true} shape. See [29] for more details.

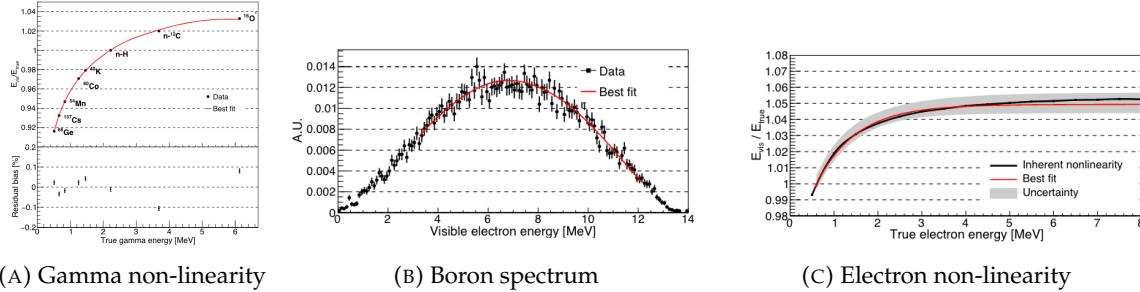


FIGURE 2.12 – Fitted and simulated non linearity of gamma, electron sources and from the ^{12}B spectrum. Black points are simulated data. Red curves are the best fits. Figures taken from [29].

2.3.2 Calibration system

The non-uniformity due to the event position in the detector (more details in section 2.6) will be studied using multiples systems that are schematized in figure 2.13. They allow to position sources at different location in the CD.

- For a one-dimension vertical calibration, the Automatic Calibration Unit (ACU) will be able to deploy multiple radioactive sources or a pulse laser diffuser ball along the central axis of the CD through the top chimney. The source position precision is less than 1cm.
- For off-axis calibration, a calibration source attached to a Cable Loop System (CLS) can be moved on a vertical half-plane by adjusting the length of two connection cable. Two set of CSL will be deployed to provide a 79% effective coverage of a vertical plane.
- A Guiding Tube (GT) will surround the CD to calibrate the non-uniformity of the response at the edge of the detector
- A Remotely Operated under-LS Vehicle (ROV) can be deployed to desired location inside LS for a more precise and comprehensive calibration. The ROV will also be equipped with a camera for inspection of the CD.

The preliminary calibration program is depicted in table 2.5.

2.3.3 Instrumental non-linearity calibration

As mentioned in the introduction of this section, we expect an instrumental non-linearity due to the LPMT system saturating. This results in the LPMT underestimating the number of collected photo-electrons. This non-linearity is illustrated in figure 2.14. This non-linearity would consequently convolve with the LS non-linearity. To correct this effect, the LPMT are first calibrated to the channel level using the dual calorimetry calibration technique which consist of comparing the LPMT and SPMT calorimetry calibration using a tunable light source covering the range of 0 to 100 PE per LPMT channel.

Within such range, the SPMT serve as an approximate linear reference since SPMT operate primarily operate in photo-counting mode in this range. Using this technique, the residual non-linearity in the LPMT response due to the saturation effect is under 0.3 %.

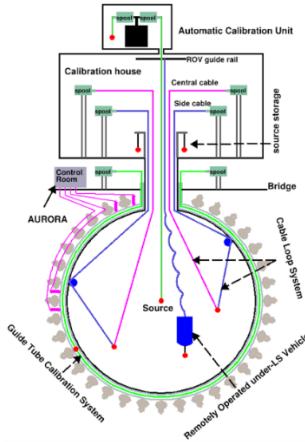


FIGURE 2.13 – Overview of the calibration system

Program	Purpose	System	Duration [min]
Weekly calibration	Neutron (Am-C)	ACU	63
	Laser	ACU	78
Monthly calibration	Neutron (Am-C)	ACU	120
	Laser	ACU	147
	Neutron (Am-C)	CLS	333
	Neutron (Am-C)	GT	73
Comprehensive calibration	Neutron (Am-C)	ACU, CLS and GT	1942
	Neutron (Am-Be)	ACU	75
	Laser	ACU	391
	^{68}Ge	ACU	75
	^{137}Cs	ACU	75
	^{54}Mn	ACU	75
	^{60}Co	ACU	75
	^{40}K	ACU	158

TABLE 2.5 – Calibration program of the JUNO experiment

2.4 Satellite detectors

As introduced in section 2.1.1 and section 2.2.2, the precise knowledge and understanding of the detector condition is crucial for the measurements of the NMO and oscillation parameters. Thus two satellite detectors will be setup to monitor the experiment condition. TAO to monitor and understand the $\bar{\nu}_e$ flux and spectrum coming from the nuclear reactor and OSIRIS to monitor the LS response.

2.4.1 TAO

The Taishan Antineutrino Observatory (TAO) [12, 30] is a ton-level gadolinium doped liquid scintillator detector that will be located near the Taishan-1 reactor. It aim to measure the $\bar{\nu}_e$ spectrum at very low distance (45m) from the reactor to measure a quasi-unoscillated spectrum. TAO also aim to provide a major contribution to the so-called reactor anomaly [13]. Its requirement are to the level of 2 % energy resolution at 1 MeV.

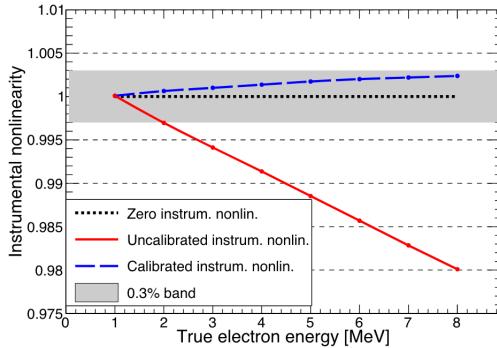


FIGURE 2.14 – Event-level instrumental non-linearity, defined as the ratio of the total measured LPMT charge to the true charge for events uniformly distributed in the detector. The solid red line represents event-level non-linearity without the channel-level correction, with position non-uniformity obtained at 1 MeV applied, in an extreme hypothetical scenario of 50% non-linearity over 100 PEs for the LPMTs. The dashed blue line represents that after the channel-level correction. The gray band shows the residual uncertainty of 0.3%, after the channel-level correction. Figure taken from [29].

478 Detector

479 The TAO detector is close, in concept, to the CD of JUNO. It is composed of an acrylic vessel
 480 containing 2.8 tons of gadolinium-loaded LS instrumented by an array of silicon photomultipliers
 481 (SiPM) reaching a 95% coverage. To efficiently reduce the dark count of those sensors, the detector
 482 is cooled to -50 °C. The $\bar{\nu}_e$ will interact with the LS via IBD, producing scintillation light, that will
 483 be detected by the SiPMs. From this signal the $\bar{\nu}_e$ energy and the full spectrum reconstructed. This
 484 spectrum will then be used by JUNO to calibrate the unoscillated spectrum, most notably the fission
 485 product fraction that impact the rate and shape of the spectrum. A schema of the detector is presented
 486 in figure 2.15a.

487 2.4.2 OSIRIS

488 The Online Scintillator Internal Radioactivity Investigation System (OSIRIS) [25] is an ultralow back-
 489 ground, 20 m³ LS detector that will be located in JUNO cavern. It aim to monitor the radioactive
 490 contamination, purity and overall response of the LS before it is injected in JUNO. OSIRIS will
 491 be located at the end of the purification chain of JUNO, monitoring that the purified LS meet the
 492 JUNO requirements. The setup is optimized to detect the fast coincidences decay of $^{214}\text{Bi} - ^{214}\text{Po}$
 493 and $^{212}\text{Bi} - ^{212}\text{Po}$, indicators of the decay chains of U and Th respectively.

494 Detector

495 OSIRIS is composed of an acrylic vessel that will contains 17t of LS. The LS is instrumented by
 496 a PMT array of 64 20 inch PMTs on the top and the side of the vessel. To reach the necessary
 497 background level required by the LS purity measurements, in addition to being 700m underground
 498 in the experiment cavern, the acrylic vessel is immersed in a tank of ultra pure water. The water is
 499 itself instrumented by another array of 20 inch PMTs, acting as muon veto. A schema of the detector
 500 is presented in figure 2.15b.

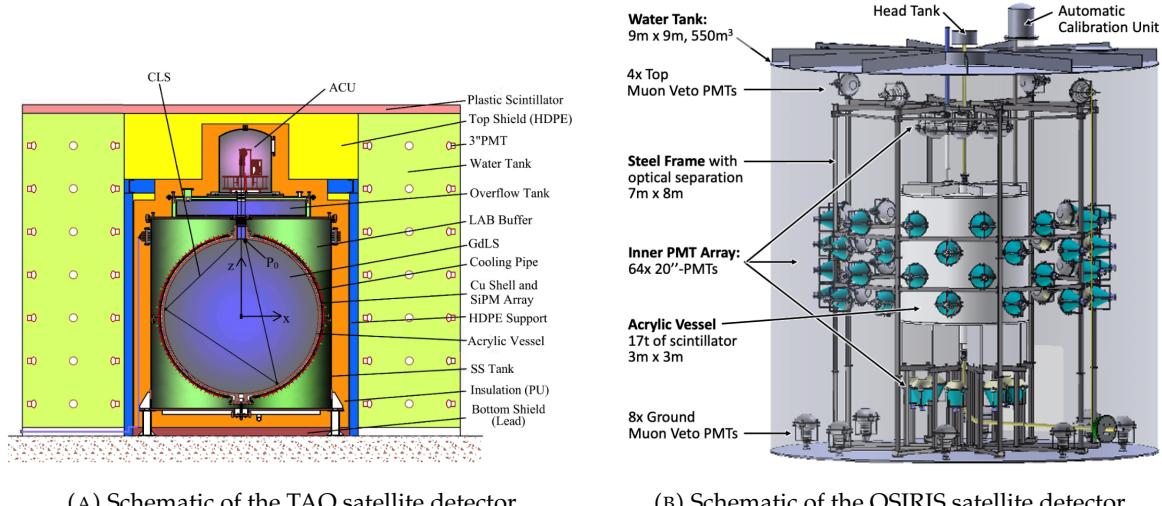


FIGURE 2.15

2.5 Software

501 The simulation, reconstruction and analysis algorithms are all packaged in the JUNO software,
 502 subsequently called the software. It is composed of multiple components integrated in the SNiPER
 503 [31] framework:

- 505 — Various primary particles simulators for the different kind of events, background and calibra-
 506 tion sources.
- 507 — A Geant4 [32–34] Monte Carlo (MC) simulation containing the detectors geometries, a custom
 508 optical model for the LS and the supporting structures of the detectors. The Geant4 simulation
 509 integrate all relevant physics process for JUNO, validated by the collaboration. This step of the
 510 simulation is commonly called *Detsim* and compute up to the production of photo-electrons
 511 in the PMTs. The optics properties of the different materials and detector components have
 512 been measured beforehand to be used to define the material and surfaces in the simulation.
- 513 — An electronic simulation, simulating the response waveform of the PMTs, tracking it through
 514 the digitization process, accounting for effects such as non-linearity, dark noise, Time Trans-
 515 it Spread (TTS), pre-pulsing, after-pulsing and ringing if the waveform. It's also the step
 516 handling the event triggers and mixing. This step is commonly referenced as *Elecsim*.
- 517 — A waveform reconstruction where the digitized waveform are filtered to remove high-frequency
 518 white noise and then deconvoluted to yield time and charge informations of the photons hits
 519 on the PMTs. This step is commonly referenced as *Calib*.
- 520 — The charge and time informations are used by reconstruction algorithms to reconstruct the
 521 interaction vertex and the deposited energy. This step is commonly reported as *Reco*. See
 522 section 2.6 for more details on the reconstruction.
- 523 — Once the singular events are reconstructed, they go through event pairing and classification
 524 to select IBD events. This step is named Event Classification.
- 525 — The purified signal is then analysed by the analysis framework which depend of the physics
 526 topic of interest.

527 The steps Reco and Event Classification are divided into two category of algorithm. Fast but less
 528 accurate algorithms that are running during the data taking designated as the *Online* algorithms.
 529 Those algorithm are used to take the decision to save the event on tape or to throw it away. More
 530 accurate algorithms that run on batch of events designated *Offline* algorithms. They are used for the
 531 physics analysis. The Offline Reco will be one of the main topic of interest for this thesis.

532 2.6 State of the art of the Offline IBD reconstruction in JUNO

533 The main reconstruction method currently run in JUNO is a data-driven method based on a like-
 534 lihood maximization [35, 36] using only the LPMTs. The first step is to reconstruct the interaction
 535 vertex from which the energy reconstruction is dependent. It is also necessary for event pairing and
 536 classification.

537 **2.6.1 Interaction vertex reconstruction**

538 To start the likelihood maximization, a rough estimation of the vertex and of the event timing is
 539 needed. We start by estimating the vertex position using a charge based algorithm.

540 **Charge based algorithm**

541 The charge-based algorithm is basically base on the charge-weighted average of the PMT position.

$$\vec{r}_{cb} = a \cdot \frac{\sum_i q_i \cdot \vec{r}_i}{\sum_i q_i} \quad (2.3)$$

542 Where q_i is the reconstructed charge of the pulse of the i th PMT and \vec{r}_i is its position. \vec{r}_0 is the
 543 reconstructed interaction position. a is a scale factor introduced because a weighted average over
 544 a 3D sphere is inherently biased. Using calibration we can estimate $a \approx 1.3$ [37]. The results in
 545 figure 2.16b shows that the reconstruction is biased from around 15m and further. This is due to the
 546 phenomena called “total reflection area” or TR Area.

547 As depicted in the figure 2.16a the optical photons, given that they have a sufficiently large incidence
 548 angle, can be deviated of their trajectories when passing through the interfaces LS-acrylic and water-
 549 acrylic due to the optical index difference. This cause photons to be lost or to be detected by PMT
 550 further than anticipated if we consider their rectilinear trajectories. This cause the charge barycenter
 551 the be located closer to the center than the event really is.

552 It is to be noted that charge based algorithm, in addition to be biased near the edge of the detector,
 553 does not provide any information about the timing of the event. Therefore, a time based algorithm
 554 needs to be introduced to provide initial values.

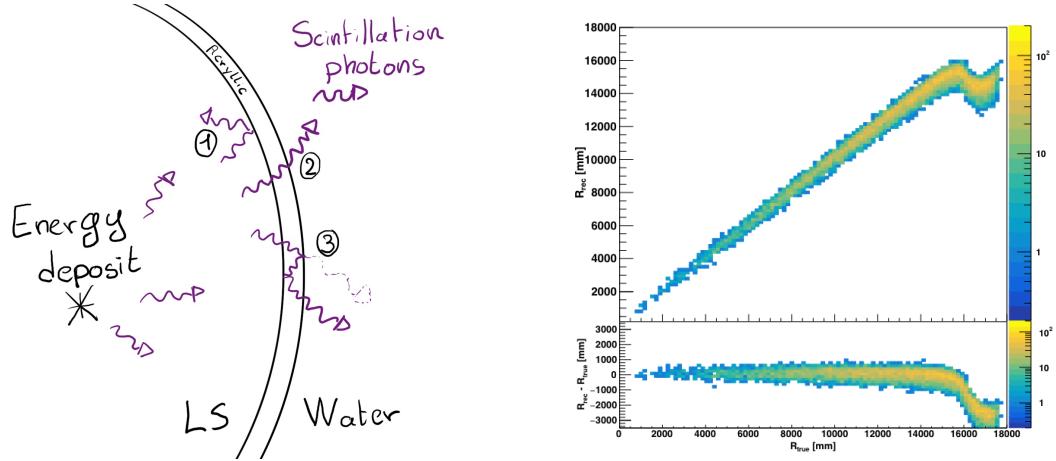
555 **Time based algorithm**

556 The time based algorithm use the distribution of the time of flight corrections Δt (Eq 2.4) of an event
 557 to reconstruct its vertex and t_0 . It follow the following iterations:

- 558 1. Use the charge based algorithm to get an initial vertex to start the iteration.
 559 2. Calculate the time of flight correction for the i th PMT using

$$\Delta t_i(j) = t_i - \text{tof}_i(j) \quad (2.4)$$

560 where j is the iteration step, t_i is the timing of the i th PMT, and tof_i is the time-of-flight of the
 561 photon considering an rectilinear trajectory and an effective velocity in the LS and water (see
 562 [37] for detailed description of this effective velocity). Plot the Δt distribution and label the
 563 peak position as Δt^{peak} (see fig 2.17a).



(A) Illustration of the different optical photons reflection scenarios. 1 is the reflection of the photon at the interface LS-acrylic or acrylic-water. 2 is the transmission of the photons through the interfaces. 3 is the conduction of the photon in the acrylic.

(B) Heatmap of R_{rec} and $R_{rec} - R_{true}$ as a function of R_{true} for 4MeV prompt signals uniformly distributed in the detector calculated by the charge based algorithm

FIGURE 2.16

564

3. Calculate a correction vector $\vec{\delta}[\vec{r}(j)]$ as

$$\vec{\delta}[\vec{r}(j)] = \frac{\sum_i \left(\frac{\Delta t(j) - \Delta t^{peak}(j)}{tof_i(j)} \right) \cdot (\vec{r}_0(j) - \vec{r}_i)}{N^{peak}(j)} \quad (2.5)$$

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568

where \vec{r}_0 is the vertex position at the beginning of this iteration, \vec{r}_i is the position of the i th PMT. To minimize the effect of scattering, dark noise and reflection, only the pulse happening in a time window (-10 ns, +5 ns) around Δt^{peak} are considered. N^{peak} is the number of PE collected in this time-window.

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570

4. if $\vec{\delta}[\vec{r}(j)] < 1\text{mm}$ or $j \geq 100$, stop the iteration. Otherwise $\vec{r}_0(j+1) = \vec{r}_0(j) + \vec{\delta}[\vec{r}(j)]$ and go to step 2.

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However because the earliest arrival time is used, t_i is related to the number photoelectrons N_i^{pe} detected by the PMT [38–40]. To reduce bias in the vertex reconstruction, the following equation is used to correct t_i into t'_i :

$$t'_i = t_i - p_0 / \sqrt{N_i^{pe}} - p_1 - p_2 / N_i^{pe} \quad (2.6)$$

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575
576
577

The parameters (p_0, p_1, p_2) were optimized to (9.42, 0.74, -4.60) for Hamamatsu PMTs and (41.31, -12.04, -20.02) for NNVT PMTs [37]. The results presented in figure 2.17b shows that the time based algorithm provide a more accurate vertex and is unbiased even in the TR area. This results (\vec{r}_0, t_0) is used as initial value for the likelihood algorithm.

578

Time likelihood algorithm

579

The time likelihood algorithm use the residual time expressed as follow

$$t_{res}^i(\vec{r}_0, t_0) = t_i - tof_i - t_0 \quad (2.7)$$

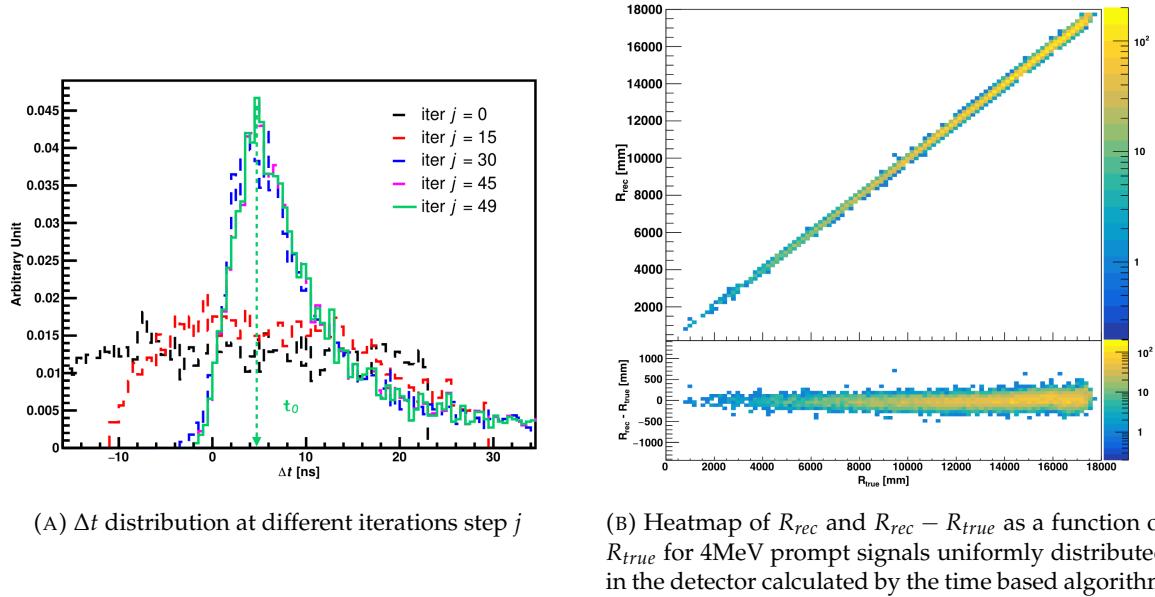


FIGURE 2.17

580 In a first order approximation, the scintillator time response Probability Density Function (PDF) can
 581 be described as the emission time profile of the scintillation photons, the Time Transit Spread (TTS)
 582 and the dark noise of the PMTs. The emission time profile $f(t_{res})$ is described like

$$f(t_{res}) = \sum_k \frac{\rho_k}{\tau_k} e^{-\frac{t_{res}}{\tau_k}}, \quad \sum_k \rho_k = 1 \quad (2.8)$$

583 as the sum of the k component that emit light in the LS each one characterised by it's decay time τ_k
 584 and intensity fraction ρ_k . The TTS component is expressed as a gaussian convolution

$$g(t_{res}) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(t_{res}-\nu)^2}{2\sigma^2}} \cdot f(t_{res}) \quad (2.9)$$

585 where σ is the TTS of PMTs and ν is the average transit time. The dark noise is not correlated with any
 586 physical events and considered as constant rate over the time window considered T . By normalizing
 587 the dark noise probability $\epsilon(t_{res})$ as $\int_T \epsilon(t_{res}) dt_{res} = \epsilon_{dn}$, it can be integrated in the PDF as

$$p(t_{res}) = (1 - \epsilon_{dn}) \cdot g(t_{res}) + \epsilon(t_{res}) \quad (2.10)$$

588 The distribution of the residual time t_{res} of an event can then be compared to $p(t_{res})$ and the best
 589 fitting vertex \vec{r}_0 and t_0 can be chosen by minimizing

$$\mathcal{L}(\vec{r}_0, t_0) = -\ln \left(\prod_i p(t_{res}^i) \right) \quad (2.11)$$

590 The parameter of Eq. 2.10 can be measured experimentally. The results shown in figure 2.18 used
 591 PDF from monte carlo simulation. The results shows that $R_{rec} - R_{true}$ is biased depending on the
 592 energy. While this could be corrected using calibration, another algorithm based on charge likelihood
 593 was developed to correct this problem.

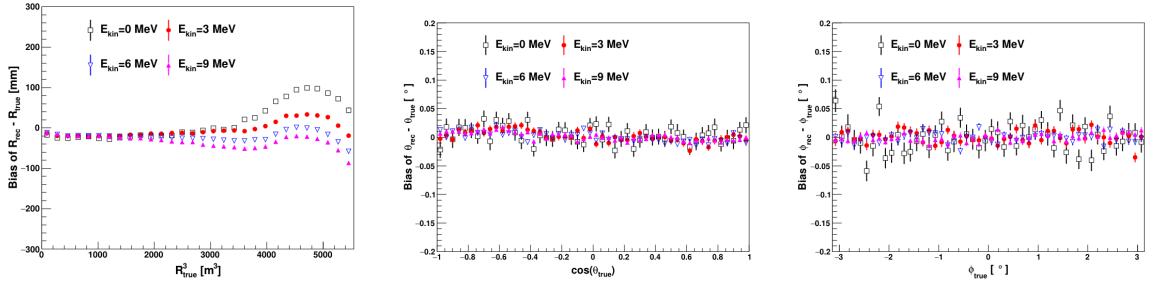


FIGURE 2.18 – Bias of the reconstructed radius R (left), θ (middle) and ϕ (right) for multiple energies by the time likelihood algorithm

594 Charge likelihood algorithm

595 Similarly to the time likelihood algorithms that use a timing PDF, the charge likelihood algorithm
 596 use a PE PDF for each PMT depending on the energy and position of the event. With $\mu(\vec{r}_0, E)$ the
 597 mean expected number of PE detected by each PMT, the probability to observe N_{pe} in a PMT follow
 598 a Poisson distribution. Thus

- 599 — The probability to observe no hit ($N_{pe} = 0$) in the j th PMT is $P_{nohit}^j(\vec{r}_0, E) = e^{-\mu_j}$
- 600 — The probability to observe $N_{pe} \neq 0$ in the i th PMT is $P_{hit}^i(\vec{r}_0, E) = \frac{\mu^{N_{pe}} e^{-\mu_i}}{N_{pe}^i!}$

601 Therefore, the probability to observe a specific hit pattern can be expressed as

$$P(\vec{r}_0, E) = \prod_j P_{nohit}^j(\vec{r}_0, E) \cdot \prod_i P_{hit}^i(\vec{r}_0, E) \quad (2.12)$$

602 The best fit values of \vec{R}_0 and E can then be calculated by minimizing the negative log-likelihood

$$\mathcal{L}(\vec{r}_0, E) = -\ln(P(\vec{r}_0, E)) \quad (2.13)$$

603 In principle, $\mu_i(\vec{r}_0, E)$ could be expressed

$$\mu_i(\vec{r}_0, E) = Y \cdot \frac{\Omega(\vec{r}_0, r_i)}{4\pi} \cdot \epsilon_i \cdot f(\theta_i) \cdot e^{-\sum_m \frac{d_m}{\zeta_m}} \cdot E + \delta_i \quad (2.14)$$

604 where Y is the energy scale factor, $\Omega(\vec{r}_0, r_i)$ is the solid angle of the i th PMT, ϵ_i is its detection
 605 efficiency, $f(\theta_i)$ its angular response, ζ_m is the attenuation length in the materials and δ_i the expected
 606 number of dark noise.

607 However Eq. 2.14 assume that the scintillation light yield is linear with energy and describe poorly
 608 the contribution of indirect light, shadow effect due to the supporting structure and the total reflec-
 609 tion effects. The solution is to use data driven methods to produce the pdf by using the calibra-
 610 tions sources and position described in section 2.3. In the results presented in figures 2.19, the PDF was
 611 produced using MC simulation and 29 specific calibrations position [37] along the Z-axis of the
 612 detector. We see that the charge likelihood algorithm show little bias in the TR area and a better
 613 resolution than the time likelihood. The figure 2.20 shows the radial resolution of the different
 614 algorithm presented for this section, we can see the refinement at each step and that the charge
 615 likelihood yield the best results.

616 The charge based likelihood algorithms already give use some information on the energy as Eq. 2.13
 617 is minimized but the energy can be further refined as shown in the next section.

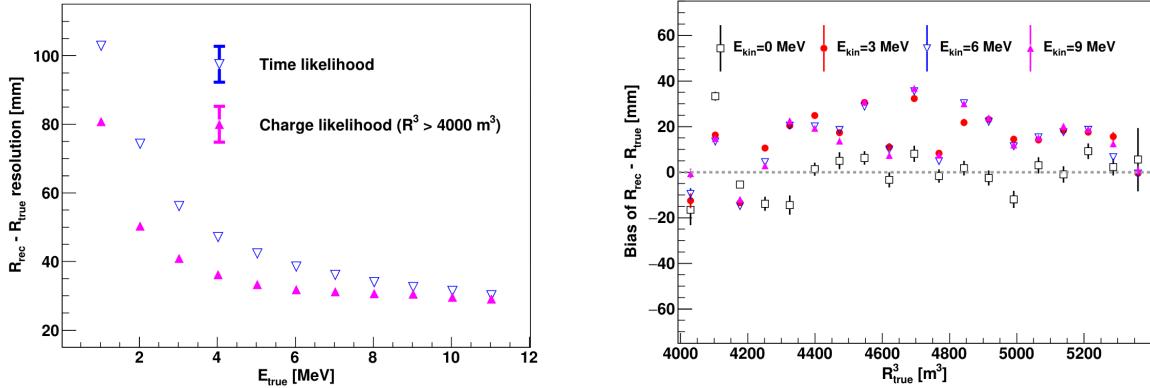


FIGURE 2.19 – On the left: Resolution of the reconstructed R as a function of the energy in the TR area ($R^3 > 4000 \text{ m}^3 \equiv R > 16 \text{ m}$) by the charge and time likelihood algorithms. On the right: Bias of the reconstructed R in the TR area for different energies by the charge likelihood algorithm

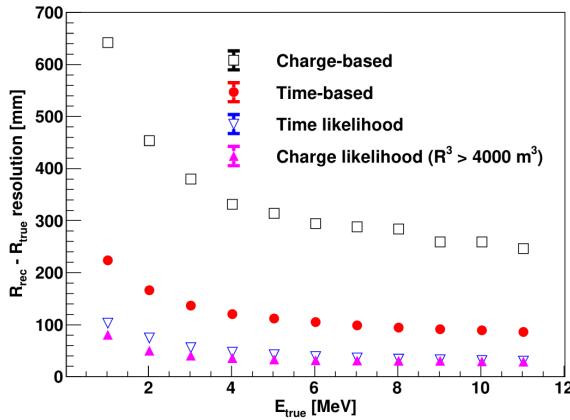


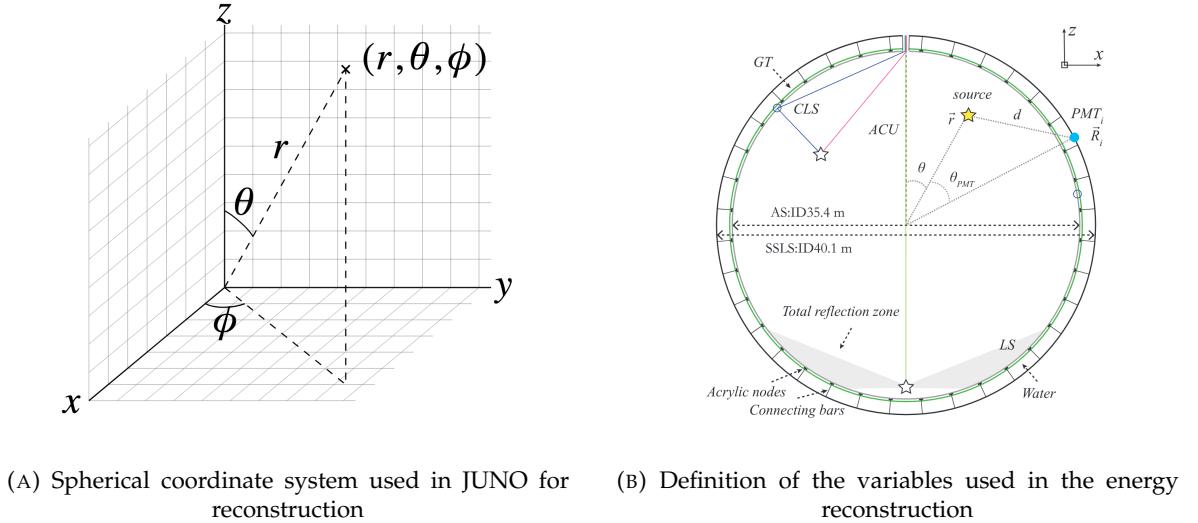
FIGURE 2.20 – Radial resolution of the different vertex reconstruction algorithms as a function of the energy

618 2.6.2 Energy reconstruction

619 As explained in section 2.1.1, energy resolution is crucial for the NMO and oscillation parameters
620 measurements. Thus the energy reconstruction algorithm should take into consideration as much
621 detector effect as possible. The following method is a data driven method based on calibration
622 samples inspired by the charge likelihood algorithm described above [41].

623 Charge estimation

624 The most important element in the energy reconstruction is $\mu_i(\vec{r}_0, E)$ described in Eq. 2.14. For
625 realistic cases, we also need to take into account the electronics effect that were omitted in the
626 previous section. Those effect will cause a charge smearing due to the uncertainties in the N_{pe}
627 reconstruction. Thus we define $\hat{\mu}^L(\vec{r}_0, E)$ which is the expected N_{pe}/E in the whole detector for an
628 event with visible energy E_{vis} and position \vec{r}_0 . The position of the event and PMTs are now defined



(A) Spherical coordinate system used in JUNO for reconstruction

(B) Definition of the variables used in the energy reconstruction

FIGURE 2.21

629 using $(r, \theta, \theta_{pmt})$ as defined in figure 2.21b.

$$\hat{\mu}(r, \theta, \theta_{pmt}, E_{vis}) = \frac{1}{E_{vis}} \frac{1}{M} \sum_i^M \frac{\bar{q}_i - \mu_i^D}{\text{DE}_i}, \quad \mu_i^D = \text{DNR}_i \cdot L \quad (2.15)$$

630 where i runs over the PMTs with the same θ_{pmt} , DE_i is the detection efficiency of the i th PMT. μ_i^D
 631 is the expected number of dark noise photoelectrons in the time window L . The time window have
 632 been optimized to $L = 280$ ns [41]. \bar{q}_i is the average recorded photoelectrons in the time window
 633 and \hat{Q}_i is the expected average charge for 1 photoelectron. The N_{pe} map is constructed following the
 634 procedure described in [36].

635 Time estimation

636 The second important observable is the hit time of photons that was previously defined in Eq. 2.7. It
 637 is here refined as

$$t_r = t_h - \text{tof} - t_0 = t_{LS} + t_{TT} \quad (2.16)$$

638 where t_h is the time of hit, t_{LS} is the scintillation time and t_{TT} the transit time of PMTs that is described
 639 by a gaussian

$$t_{TT} = \mathcal{N}(\bar{\mu}_{TT} + t_d, \sigma_{TT}) \quad (2.17)$$

640 where μ_{TT} is the mean transit time in PMTs, σ_{TT} is the Transit Time Spread (TTS) of the PMTs and t_d
 641 is the delay time in the electronics. The effective refraction index of the LS is also corrected to take
 642 into account the propagation distance in the detector.

643 The timing PDF $P_T(t_r | r, d, \mu_l, \mu_d, k)$ can now be generated using calibration sources [41]. This PDF
 644 describe the probability that the residual time of the first photon hit is in $[t_r, t_r + \delta]$ with r the radius
 645 of the event vertex, $d = |\vec{r} - \vec{r}_{PMT}|$ the propagation distance, μ_l and μ_d the expected number of PE
 646 and dark noise in the electronic reading window and k is the detected number of PE.

647 Now let denote $f(t, r, d)$ the probability density function of "photoelectron hit a time t" for an event

648 happening at r where the photons traveled the distance d in the LS

$$F(t, r, d) = \int_t^L f(t', r, d) dt' \quad (2.18)$$

649 Based on the PDF for one photon $k = 1$, one can define

$$P_T^l(t|k = n) = I_n^l [f_l(t) F_l^{n-1}(t)] \quad (2.19)$$

650 where the indicator l means that the photons comes from the LS and I_n^l a normalisation factor. To this
651 pdf we add the probability to have photons coming from the dark noise indicated by the indicator d
652 using

$$f_d(t) = 1/L, F_d(t) = 1 - \frac{t}{L} \quad (2.20)$$

653 and so for the case where only one photon is detected by the PMT ($k = 1$)

$$P_T(t|\mu_l, \mu_d, k = 1) = I_1[P(1, \mu_l)P(0, \mu_d)f_l(t) + P(0, \mu_l)P(1, \mu_d)f_d(t)] \quad (2.21)$$

654 where $P(k_\alpha, \mu_\alpha)$ is the Poisson probability to detect k_α PE from $\alpha \in \{l, d\}$ with the condition $k_l + k_d =$
655 k .

656 Now that we have the individual timing and charge probability we can construct the charge likeli-
657 hood referred as QMLE:

$$\mathcal{L}(q_1, q_2, \dots, q_N | \vec{r}, E_{vis}) = \prod_{j \in \text{unfired}} e^{-\mu_j} \prod_{i \in \text{fired}} \left(\sum_{k=1}^K P_Q(q_i|k) \cdot P(k, \mu_i) \right) \quad (2.22)$$

658 where $\mu_i = E_{vis}\hat{\mu}_i^L + \mu_i^D$ and $P(k, \mu_i)$ is the Poisson probability of observing k PE. $P_Q(q_i|k)$ is the
659 charge pdf for k PE. And we can also construct the time likelihood referred as TMLE:

$$\mathcal{L}(t_{1,r}, t_{2,r}, \dots, t_{N,r} | \vec{r}, t_0) = \prod_{i \in \text{hit}} \frac{\sum_{k=1}^K P_T(t_{i,r}|r, d, \mu_i^l, \mu_i^d, k) \cdot P(k, \mu_i^l + \mu_i^d)}{\sum_{k=1}^K P(k, \mu_i^l + \mu_i^d)} \quad (2.23)$$

660 where K is cut to 20 PE and hit is the set of hits satisfying $-100 < t_{i,r} < 500$ ns.

661 Merging those two likelihood give the charge-time likelihood QTMLE

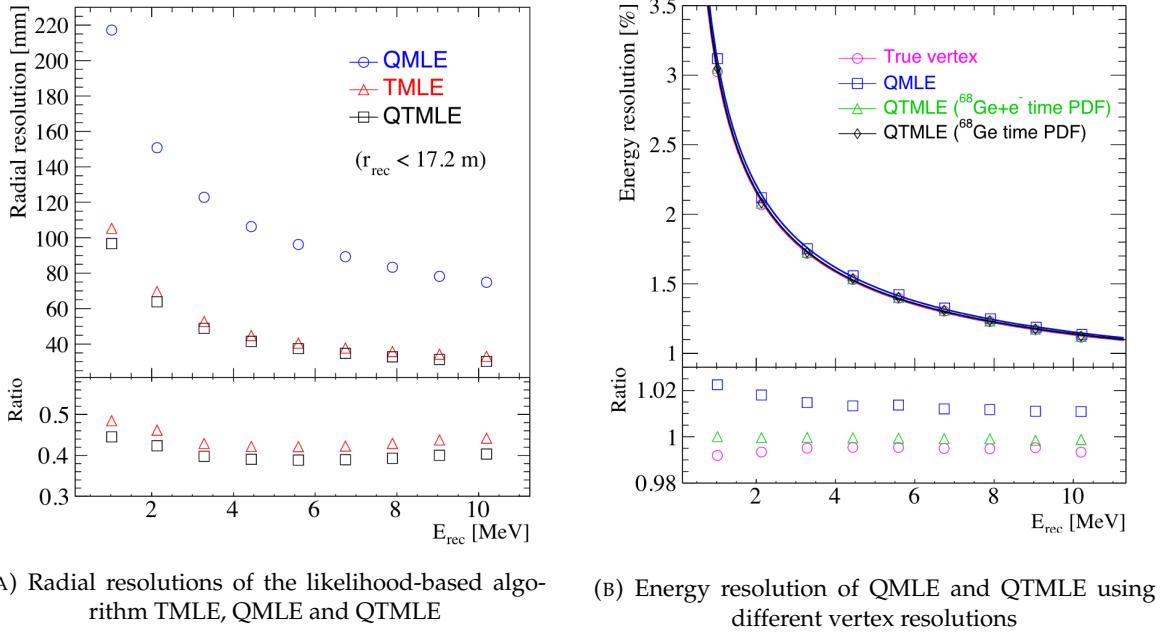
$$\mathcal{L}(q_1, q_2, \dots, q_N; t_{1,r}, t_{2,r}, \dots, t_{N,r} | \vec{r}, t_0, E_{vis}) = \mathcal{L}(q_1, q_2, \dots, q_N | \vec{r}, E_{vis}) \cdot \mathcal{L}(t_{1,r}, t_{2,r}, \dots, t_{N,r} | \vec{r}, t_0) \quad (2.24)$$

662 The radial and energy resolutions of the different likelihood are presented in figure 2.22 (from [41]).
663 We can see the improvement of adding the time information to the vertex reconstruction and that
664 an increase in vertex precision can bring improvement in the energy resolution, especially at low
665 energies.

666 Data driven methods prove to be performant in the energy and vertex reconstruction given that we
667 have enough calibrations sources to produce the PDF. In the next section, we'll see another type of
668 data-driven method based on machine learning.

669 2.6.3 Machine learning for reconstruction

670 Machine learning (ML) is family of data-driven algorithms that are inferring behavior and results
671 from a training dataset. A overview of methods and detailed explanation of the Neural Network
672 (NN) subfamily can be found in Chapter 3.



(B) Energy resolution of QMLE and QTML using different vertex resolutions

FIGURE 2.22

673 The power of ML is the ability to model complex response to a specific problem. In JUNO the
 674 reconstruction problematic can be expressed as follow: knowing that each PMT, large or small,
 675 detected a given number of PE Q at a given time t and their position is x, y, z where did the energy
 676 was deposited and how much energy was it, modeling a function that naively goes:

$$\mathbb{R}^{5 \times N_{\text{pmt}}} \mapsto \mathbb{R}^4 \quad (2.25)$$

677 It is worth pointing that while this is already a lot in informations, this is not the rawest representa-
 678 tion of the experiment. We could indeed replace the charge and time by the waveform in the time
 679 window of the event but that would lead to an input representation size that would exceed our
 680 computational limits. Also, due to those computational limits, most of the ML algorithm reduce this
 681 input phase space either by structurally encoding the information (pictures, graph), by aggregating
 682 it (mean, variance, ...) or by exploiting invariance and equivariance of the experiment (rotational
 683 invariance due to the sphericity, ...).

684 For machine learning to converge to performant algorithm, a large dataset exploring all the phase
 685 space of interest is needed. For the following studies, data from the monte carlo simulation presented
 686 in section 2.5 are used for training. When the detector will be finished calibrations sources will be
 687 complementarily be used.

688 **Boosted Decision Tree (BDT)**

689 On of the most classic ML method used in physics in last years is the Boosted Decision Tree (see
 690 chapter 3.1). They have been explored for vertex reconstruction [42] et for energy reconstruction [42,
 691 43].

692 For vertex and energy reconstruction a BDT was developed using the aggregated informations pre-
 693 sented in 2.6.

694 Its reconstruction performances are presented in figure 2.24.

Parameter	description
$nHits$	Total number of hits
$x_{cc}, y_{cc}, z_{cc}, R_{cc}$	Coordinates of the center of charge
ht_{mean}, ht_{std}	Hit time mean and standard deviation

TABLE 2.6 – Features used by the BDT for vertex reconstruction

AccumCharge	$ht_{5\% - 2\%}$
R_{cht}	pe_{mean}
z_{cc}	J_{cht}
pe_{std}	ϕ_{cc}
nPMTs	$ht_{35\% - 30\%}$
$ht_{kurtosis}$	$ht_{20\% - 15\%}$
$ht_{25\% - 20\%}$	$pe_{35\%}$
R_{cc}	$ht_{30\% - 25\%}$

TABLE 2.7 – Features used by the BDTE algorithm. pe and ht reference the charge and hit-time distribution respectively and the percentages are the quantiles of those distributions. cht and cc reference the barycenters of hit time and charge respectively

695 A second and more advanced BDT, subsequently named BDTE, that only reconstruct energy use a
 696 different set of features [43]. They are presented in the table 2.7

697 Neural Network (NN)

698 The physics have shown a rising for Neural Network (NN) in the past years for event reconstruction,
 699 notably in the neutrino community [44–47]. Three type of neural networks have explored for event
 700 reconstruction in JUNO Deep Neural Network (DNN), Convolutional Neural Network (CNN) and
 701 Graph Network (GNN). More explanation about those neural network can be found in chapter 3.

702 The CNN are using 2D projection of the detector representing it as an image with two channel, one
 703 for the charge Q and one for the time t . The position of the PMTs is structurally encoded in the pixel
 704 containing the information of this PMT. In [42], the pixel is chosen based on a transformation of θ
 705 and ϕ coordinates to the 2D plane and rounded to the nearest pixel. A sufficiently large image has
 706 been chosen to prevent two PMT to be located in the same pixel. An example of this projection can
 707 be found in figure 2.23. The performances of the CNN can be found in figure 2.24.

708 Using 2D have the upside of encoding a large part of the informations structurally but loose the rotational
 709 invariance of the detector. It also give undefined information to the neural network (what is a
 710 pixel without PMT ? What should be its charge and time ?), cause deformation in the representation
 711 of the detector (sides of projection) and loose topological informations.

712 One of the way to present structurally the sphericity of JUNO to a NN is to use a graph: A collection
 713 of objects V called nodes and relations E called edges, each relation associated to a couple v_1, v_2
 714 forming the graph $G(E, V)$. Nodes and edges can hold informations or features. In [42] the nodes,
 715 are geometrical region of the detector as defined by the HealPix [48]. The features of the nodes are
 716 aggregated informations from the PMTs it contains. The edges contains geographic informations of
 717 the nodes relative positions.

718 This data representation has the advantages to keep the topology of the detector intact. It also permit
 719 the use of rotational invariant algorithms for the NN, thus taking advantage of the symmetries of the
 720 detector.

721 The neural network then process the graph using Chebyshev Convolutions [49]. The performances
 722 of the GNN are presented in figure 2.24.

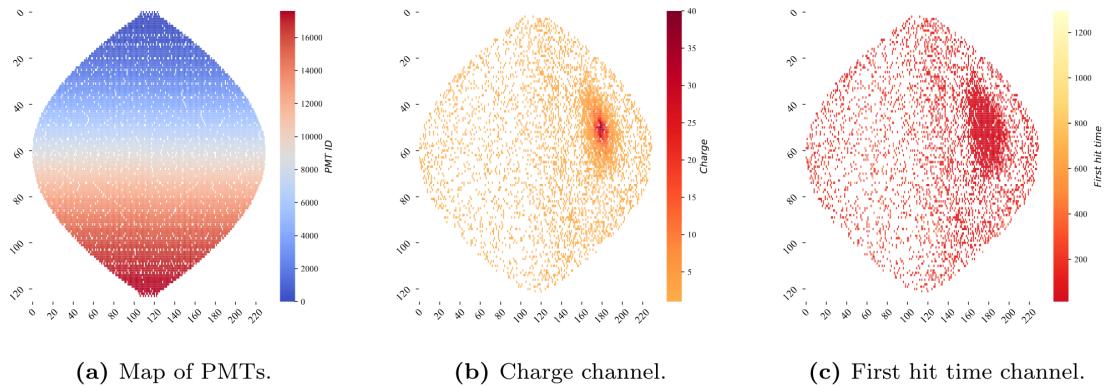


FIGURE 2.23 – Projection of the LPMTs in JUNO on a 2D plane. (a) Show the distribution of all PMTs and (b) and (c) are example of what the charge and time channel looks like respectively

Overall ML algorithms show similar performances as classical algorithms in term of energy reconstructions with the more complex structure CNN and GNN showing better performances than BDT and DNN. For vertex reconstruction, the BDT and DNN show poor performance while CNN are on the level of the classical algorithms.

2.7 JUNO sensitivity to NMO and precise measurements

Now that the event have been reconstructed, selected and that the non-IBD background have been rejected, we have access to the measured energy flux from JUNO. We consider two spectra, the one measured by the LPMT system and the one measured by the SPMT system. This give rise to three possible analysis: A LPMT only analysis, a SPMT only analysis and a joint analysis. This joint analysis is the subject of the chapter 7 of this thesis.

The following details about JUNO measurement is common to the three analysis. The details and specific of the joint analysis are detailed in chapter 7.

2.7.1 Theoretical spectrum

To extract the oscillation parameters and the NMO from the measured spectrum, it is compared to a theoretical spectrum. This theoretical spectrum is produced based on the theory of the three flavour oscillation (see section 1.3), the measurements produced by the calibration, the input from TAO and adjusted Monte Carlo simulations:

- The absolute flux and the fission product fraction yield calibrated by TAO.
 - The estimation of the neutrinos flux from other sources, such as the geoneutrinos, by theoretical model.
 - The computed cross-section of $\bar{\nu}_e$ and the LS.
 - The estimation of mislabelled event, such as fast neutron events from cosmic muons, using Monte Carlo simulation.
 - The measured bias and resolution of the LPMT and SPMT system by the calibration.
 - The time dependent reactor parameters (age of fuel, instantaneous power of the reactors, etc...)
- These systematics parameters come with their uncertainties that need to be taken into account by the fitting framework. This theoretical spectrum will, in the end, depend of the oscillation parameters of

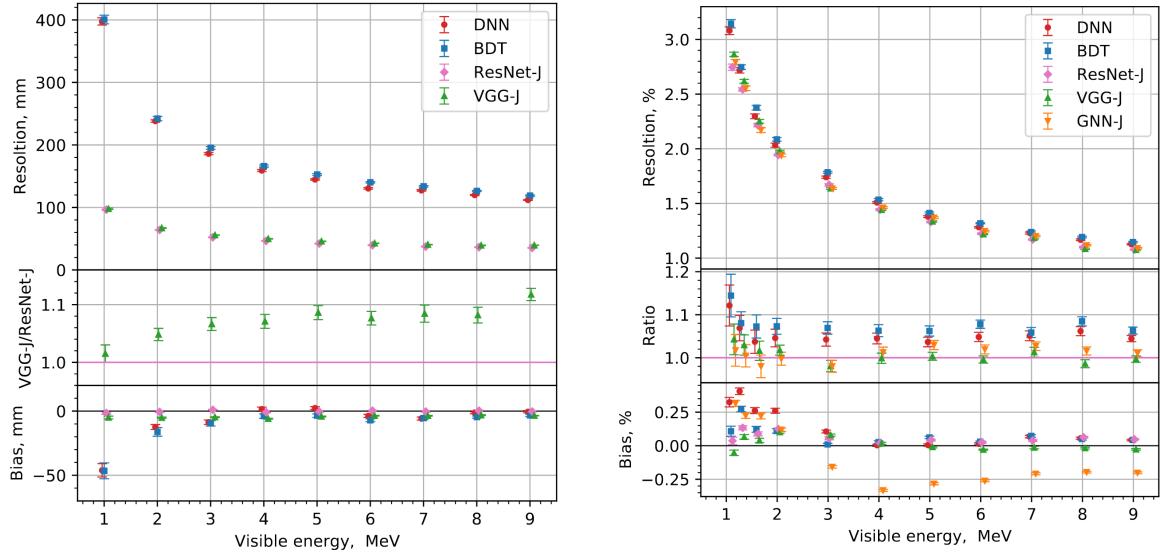


FIGURE 2.24 – Radial (left) and energy (right) resolutions of different ML algorithms. The results presented here are from [42]. DNN is a deep neural network, BDT is a BDT, ResNet-J and VGG-J are CNN and GNN-J is a GNN.

interest $\theta_{13}, \theta_{12}, \Delta m_{21}^2, \Delta m_{31}^2$. Noise parameters can be included in the parameters spectrum such as the earth density ρ between the power plants and JUNO.

2.7.2 Fitting procedure

The theoretical and measured spectra are represented as two histograms depending on the energy. The theoretical spectrum is adjusted with the data using a χ^2 minimization where χ^2 is naively defined as

$$\chi^2 = \sum_i \frac{(N_{th}^i - N_{data}^i)^2}{\sigma_i^2} \quad (2.26)$$

where N_{th}^i is the number event in the i th bin of the theoretical spectrum, N_{data}^i is the number of event in the i th bin of the measured spectrum and σ_i is the uncertainty of this bin. Two classic statistic test exist Pearson and Neyman where the difference is the estimation of σ_i parameters.

This σ_i is composed of the systematics uncertainties discussed above but also from the statistic uncertainty of the spectrum. Considering a Poisson process, the statistic uncertainty is estimated as $\sigma_{stat}^i = \sqrt{N^i}$. In a Pearson test, $N^i \equiv N_{th}^i$ whereas in a Neyman test $N^i \equiv N_{data}^i$. Under the assumption that the content of each bin follow a Gaussian distribution (a Poisson with high enough statistic), the two test are equivalent. But studies on Monte Carlo spectrum showed that the Pearson and Neyman statistic are biased in opposite direction. It is easily visible where, for the same data, Pearson will prefer a higher N_{th}^i to reduce the ration $\frac{1}{N_{th}^i}$ whereas Neyman will prefer a lower N_{th}^i to reduce the $(N_{th}^i - N_{data}^i)$ term.

This problematic can be circumvented by summing the two test, yielding the CNP statistic test and/or by adding a term

$$\chi^2 = \sum_i \frac{(N_{th}^i - N_{data}^i)^2}{\sigma_i^2} - \ln |\mathbf{V}| \quad (2.27)$$

where V is the covariance matrix of the theoretical spectrum yielding the PearsonV and CNPV

⁷⁷⁰ statistic test.

⁷⁷¹ The χ^2 is minimized by exploring the parameter phase space via gradient descent.

⁷⁷² 2.7.3 Physics results

⁷⁷³ The oscillation parameters are directly extracted from the minimization procedure and the error can
⁷⁷⁴ be estimated directly from the procedure. For the NMO, the data are fitted under the two assumption
⁷⁷⁵ of NO and IO. The difference in χ^2 give us the preferred ordering and the significance of our test.
⁷⁷⁶ Latest studies show that the precision on oscillation parameters after six year of data taking will be
⁷⁷⁷ of 0.2%, 0.3%, 0.5% and 12.1% for Δm_{31}^2 , Δm_{21}^2 , $\sin^2 \theta_{12}$ and $\sin^2 \theta_{13}$ respectively [11]. The expected
⁷⁷⁸ sensitivity to mass ordering is 3σ after 6 years [50].

⁷⁷⁹ 2.8 Summary

⁷⁸⁰ JUNO is one the biggest new generation neutrino experiment. Its goal, the measurements of oscil-
⁷⁸¹ lation parameters with unprecedented precision and an NMO preference at the 3 sigma confidence
⁷⁸² level, needs an in depth knowledge and understanding of the detector and the physics at hand. The
⁷⁸³ characterisation and calibration of the detector are of the utmost importance and the understanding
⁷⁸⁴ of the detector response in its resolution and bias is capital to be able to correctly carry the high
⁷⁸⁵ precision physics analysis of the neutrino oscillation.

⁷⁸⁶ In this thesis, I explore the usage of data-driven reconstruction methods to validate and optimize the
⁷⁸⁷ reconstruction of IBD events in JUNO in the chapters 4, 5 and 6 and the usage of the dual calorimetry
⁷⁸⁸ in the detection of possible mis-modelisation in the theoretical spectrum 7.

⁷⁸⁹ **Chapter 3**

⁷⁹⁰ **Machine learning and Artificial
Neural Network**

⁷⁹² *"I have the shape of a human being and organs equivalent to those of a human being. My organs, in fact, are identical to some of those in a prostheticized human being. I have contributed artistically, literally, and scientifically to human culture as much as any human being now alive. What more can one ask?"*

Isaac Asimov, *The Complete Robot*

⁷⁹³ Machine Learning (ML) and more specifically Neural Network (NN) are families of data-driven ⁷⁹⁴ algorithm. They are used to model complex distributions from a finite dataset to extract a generalist ⁷⁹⁵ behavior. They learn, adapt their intrinsic parameters, interactively by computing its performance ⁷⁹⁶ or loss on those dataset. They take advantage of simple microscopic operation such as *if condition* or ⁷⁹⁷ non-continuous but differentiable function like *ReLU*. Through optimizers and the combination of a ⁷⁹⁸ lot of those microscopic operations, they can obtain complex and precise behaviours.

⁷⁹⁹ They are now widely used in a wide variety of domain including natural language processing, ⁸⁰⁰ computer vision, speech recognition and, the subject of this thesis, scientific studies.

⁸⁰¹ We found them in particle physics, either as the main algorithm or as secondary algorithm, for event ⁸⁰² reconstruction, event classification, waveform reconstruction, etc..., domains where the underlying ⁸⁰³ physic and detector process is complex and highly dimensional. Physicists have traditionally been ⁸⁰⁴ forced to use simplifications or assumptions to ease the development of algorithms or equations ⁸⁰⁵ (a good example is the algorithm presented in section 2.6) where machine learning could refine and ⁸⁰⁶ take into account those effects, provided that they have enough data and computing power.

⁸⁰⁷ This chapter present an overview of the different kind of machine learning methods and neural ⁸⁰⁸ networks that will be discussed in this thesis.

⁸⁰⁹ **3.1 Boosted Decision Tree (BDT)**

⁸¹⁰ One of the most classic machine learning algorithm used in particle physics is Boosted Decision Tree ⁸¹¹ (BDT) [51] (or more recently Gradient Boosting Machine [52]). The principle of a BDT is fairly simple ⁸¹² : based on a set of observables, a serie of decisions, represented as node in a tree, are taken by the ⁸¹³ algorithm. Each decision point, or node, takes its decision based on a set of trainable parameters ⁸¹⁴ leading to a subtree of decision. The process is repeated until it reach the final node, yielding the ⁸¹⁵ prediction. A simplistic example is given in figure 3.1.

⁸¹⁶ The training procedure follow a simple score reward procedure. During the training phase the ⁸¹⁷ prediction of the BDT is compared to a known truth about the data. The score is then used to

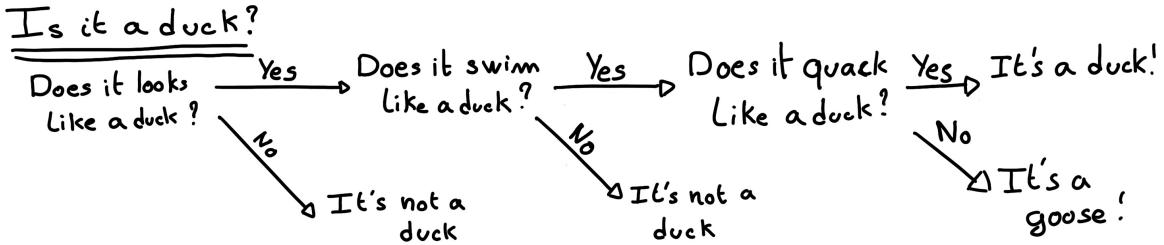


FIGURE 3.1 – Example of a BDT that determine if the given object is a duck

818 backpropagate corrections to the parameters of the tree. Modern BDT use gradient boosting where
 819 the gradient of the loss is calculated for each of the BDT parameters. Following the gradient descent,
 820 we can reach the, hopefully, global minima of the loss for our set of parameters.

821 3.2 Artificial Neural Network (NN)

822 One other big family of machine learning algorithm is the artificial Neural Networks (NN). The idea
 823 of developing automates which component mimic, in a simplistic way, the behavior of biological
 824 neurons emerge in 1959 with the paper “*What the Frog’s Eye Tells the Frog’s Brain*” [53]. They develop
 825 an automate where each component possess an *activation function*. Each one of those component then
 826 transmit its information to the other following a certain efficiency or *weight*. Those works influenced
 827 scientist and notably Frank Rosenblatt who published in 1958 what is considered the first neural
 828 network model the Perceptron [54].

829 Modern neural network still nowadays use the neuron metaphor to represent neural network, but
 830 approach them as a graph where the nodes are neurons possessing an activation function and edges
 831 holding the weights, or *parameters* in modern literature, between those nodes. Most of the modern
 832 neural network work with the principle of neurons layers. Each neurons belong to a layer and takes
 833 input from the preceding layer and forward it result to next layer. For example the most basic set
 834 layer is the fully connected layer where each of its neurons is connected to every other neurons of
 835 the precessing layer. All the neurons posses the same activation function F . The connection between
 836 two the two layers is expressed as a tensor T_j^i where i is the index of the precedent layer and j the
 837 index of the current layer. The propagation from the layer I to J is then described as

$$J_j = F_j(T_j^i I_i + B_j) \quad (3.1)$$

838 where the learning parameters are the tensor T_j^i and the bias tensor B_j . This is the fundamental
 839 component of the Fully Connected Deep NN (FCDNN) family presented in section 3.2.1. Most of the
 840 modern neural networks use gradient descent to optimize their parameters, i.e. the gradient of the
 841 parameter θ in respect of the loss function \mathcal{L} is subtracted to it

$$\theta_{i+1} = \theta_i - \frac{\partial \mathcal{L}}{\partial \theta} \quad (3.2)$$

842 i being the training iteration index. This needs the expression of \mathcal{L} dependent of θ to be differentiable,
 843 thus the layer and their activation function also need to be differentiable. This simple gradient
 844 descent, designated as Stochastic Gradient Descent (SGD), can be completed with first and second
 845 order momentum like with the Adam optimizer [55] (more details in section 3.2.5).

846 This description of neural networks as layer introduced the principle of *depth* and *width*, the number
 847 of layers in the NN and the number of neurons in each layer respectively. Those quantities that not

848 directly used for the computation of the results but describe the NN or its training are designated as
 849 *hyperparameters*.

850 The loss \mathcal{L} described above is a score representing how well the NN is doing. As seen above, it
 851 needs to be differentiable with respect to the parameter of the NN. Depending if we try to minimize
 852 or maximize it, it need to posses a minima or a maxima. For example when doing *regression*, i.e.
 853 produce a scalar result, a common loss is the Mean Square Error (MSE). Let i be our dataset, y_i be the
 854 target scalar, x_i the input data and $f(x_i, \theta)$ the result of the network. The network here is modelled by
 855 f , and its parameter by the set

$$\mathcal{L} := MSE = \frac{1}{N} \sum_i^N (y_i - f(x_i))^2 \quad (3.3)$$

856 Another common loss function is the Mean Absolute Error (MAE)

$$\mathcal{L} := MAE = \frac{1}{N} \sum_i^N |y_i - f(x_i)| \quad (3.4)$$

857 3.2.1 Fully Connected Deep Neural Network (FCDNN)

858 Fully Connected Deep Neural Network (FCDNN) architecture is the natural evolution of the Perceptron.
 859 The input data is represented as a first order tensor I_j and then fed forward to multiple fully
 860 connected layers (Eq 3.1) as presented in the figure 3.2a. Most of the time, the classic ReLU function

$$\text{ReLU}(x) = \begin{cases} x & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases} \quad (3.5)$$

861 is used as activation function. Prelu and Sigmoid are also popular choices:

$$\text{Sigmoid}(x) = \frac{1}{1 + e^{-x}} \quad (3.6) \quad \text{PReLU}(x) = \begin{cases} x & \text{if } x \geq 0 \\ \alpha x & \text{otherwise} \end{cases} \quad (3.7)$$

863 The reasoning behind ReLU and PReLU is that with enough of them, you can mimic any continuous
 864 function as illustrated in figure 3.2b. Sigmoid is more used in case of classification, its behavior going
 865 hand in hand with the Cross Entropy loss function used in classification problems.

866 Due to its simplicity, FCDNN are also used as basic pieces for more complex architectures such as
 867 the CNN and GNN that will be presented in the next section.

868 3.2.2 Convolutional Neural Network (CNN)

869 Convolutional Neural Networks are a family of neural networks that use discrete convolution filters,
 870 as illustrated in an example in figure 3.3, to process the input data, often images. They have the
 871 advantage to be translation invariant by construction, this mean that they are capable of detecting
 872 oriented features independently of their location on the image. The learning parameters are located
 873 in the filters, the network thus learn the optimal filters to extract the desired features. 2D CNN,
 874 where the filters are second order tensors that span over third order tensors, are commonly used in
 875 image recognition [56] for classification or regression problematics.

876 The convolution layers are commonly chained [57], reducing the input dimension while increasing
 877 the number of filters. The idea behind is that the first layers will process local informations and the
 878 latest layers will process more global informations. To try to preserve the amount of information, we
 879 tend to double the numbers of filters for each division of the input data. The results of the convolution

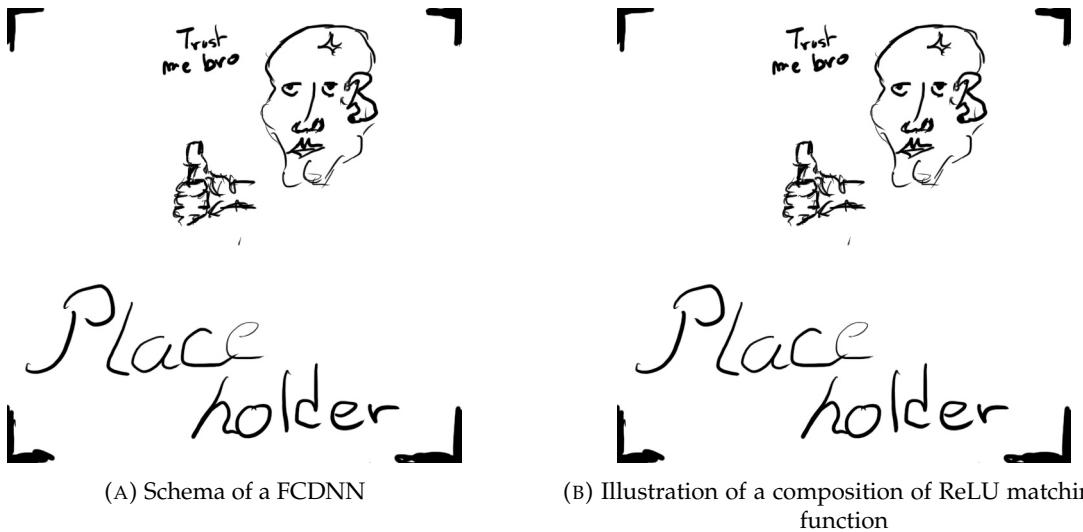


FIGURE 3.2

filters is commonly then flattened and feed to a smaller FCDNN which will process the filters results to yield the desired output.

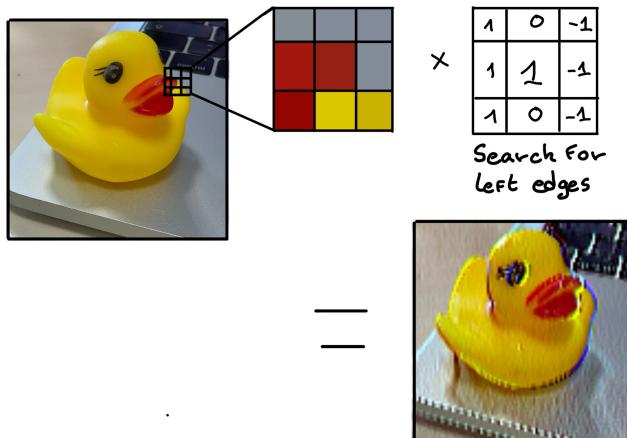


FIGURE 3.3 – Illustration of the effect of a convolution filter. Here we apply a filter with the aim do detect left edges. We see in the resulting image that the left edges of the duck are bright yellow where the right edges are dark blue indicating the contour of the object. The convolution was calculated using [58].

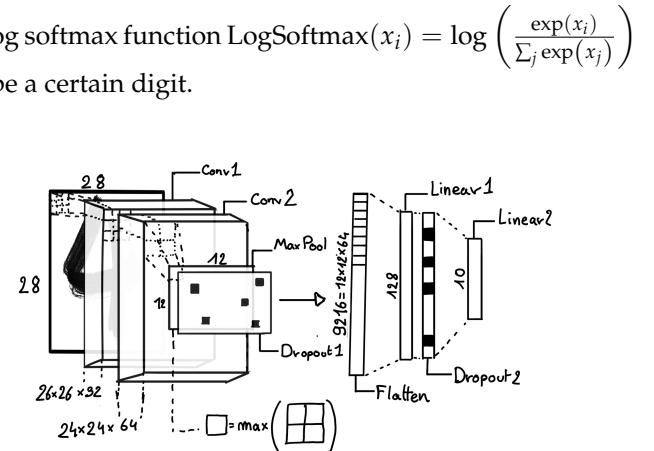
As an example, let's take the Pytorch [59] example for the MNIST [60], a dataset of black and white images of handwritten digits. Those images are 28×28 pixels with only one channel corresponding to the grey level of the pixel. Example of images from this dataset are presented in figure 3.4a

A schema of the CNN used in the Pytorch example is presented in figure 3.4b. Using this schema as a reference, the trained network is made of:

1. A convolutional layer of (3×3) filters yielding 32 channels. A bias parameter is applied to each channel for a total of $(32 \cdot (3 \times 3) + 32) = 320$ parameters. The resulting image is $(26 \times 26 \times 32)$ (26 per 26 pixels with 32 channels). The ReLU activation function is applied to each pixel.
2. A second convolutional layer of (3×3) filters yielding 64 channels. This channel also posses

- 892 a bias parameter for a total of $(64 \cdot (3 \times 3) + 64) = 640$ parameters. Resulting image is $(24 \times$
 893 $24 \times 64)$. Also with with a ReLU activation function.
- 894 3. Then comes a (2×2) max pool layer with a stride of 1 meaning that for each channel the max
 895 value of pixels in a (2×2) block is condensed in a single resulting pixel. The resulting image
 896 is $(12 \times 12 \times 64)$.
- 897 4. This image goes through a dropout layer which will set the pixel to 0 with a probability of
 898 0.25. This help prevent overtraining of the neural network (see section 3.2.6 for more details).
- 899 5. The data is the flattened i.e. condensed into a vector of $(12 \times 12 \times 64) = 9216$ values.
- 900 6. Then comes a fully connected linear layer (Eq. 3.1) with a ReLU activation that output 128
 901 feature. It needs $(9216 \cdot 128) + 128 = 1'179'776$ parameters.
- 902 7. This 128 item vector goes through another dropout layer with a probability of 0.5
- 903 8. The vector is then transformed through a linear layer with ReLU activation. It output 10
 904 values, one for each digit class $(0, 1, 2, \dots, 9)$. It need $(128 \cdot 10) + 128 = 1408$ parameters.
- 905 9. Finally the 10 values are normalized using a log softmax function $\text{LogSoftmax}(x_i) = \log \left(\frac{\exp(x_i)}{\sum_j \exp(x_j)} \right)$
 906 to give the probability of the input image to be a certain digit.

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9



(A) Example of images in the MNIST dataset

(B) Schema of the CNN used in Pytorch example to process the MNIST dataset

FIGURE 3.4

907 The final network needs 1'182'144 parameters or, if we consider each parameters to be a double
 908 precision floating point, 9.45 MB of data. To gives a order of magnitude, such neural network is
 909 considered "simple", train in a matter of minutes on T4 GPU [61] (14 epochs) and reach an accuracy
 910 in its prediction of 99%.

911 3.2.3 Graph Neural Network (GNN)

912 Graph neural network is a family of neural network where the data is represented as a graph $G(\mathcal{N}, \mathcal{E})$
 913 composed of vertex or node $n \in \mathcal{N}$ and edges $e \in \mathcal{E}$. The edges are associated to two nodes $(u, v) \in$
 914 \mathcal{N}^2 , "connecting" them. The node and the edges can hold features, commonly represented as vector
 915 $n \in \mathbb{R}^{k_n}$, $e \in \mathbb{R}^{k_e}$. We can thus define a graph using two tensors A_e^{ij} the adjacency tensors that hold
 916 the features e of the edge connecting the node i and j and the tensor N_v^i that hold the features v of a
 917 node i .

918 To efficiently manipulate such object we need to structurally encode their property in the neural
 919 network architecture: each node is equivalent (as opposite to ordered data in a vector), each node has
 920 a set of neighbours, ... One of this method is the message passing algorithm presented historically

921 in “Neural Message Passing for Quantum Chemistry” [62]. In this algorithm, with each layer of
 922 message passing a new set of features is computed for each node following

$$n_i^{k+1} = \phi_u(n_i^k, \square_j \phi_m(n_i^k, n_j^k, e_{ij}^k)); n_j \in \mathcal{N}'_i \quad (3.8)$$

923 where ϕ_u is a differentiable update function, \square_j is a differentiable aggregation function and ϕ_m is a
 924 differentiable message function. $\mathcal{N}'_i = \{n_j \in \mathcal{N} | (n_i, n_j) \in \mathcal{E}\}$ is the set of neighbours of n_i , i.e. the
 925 nodes n_j from which it exist an edge $e_{i,j} \rightarrow (n_i, n_j)$. k is the layer on which the message passing
 926 algorithm is applied. \square need also a few other property if we want to keep the graph property, most
 927 notably the permutational invariance of its parameters (example: mean, std, sum, ...).

928 The edges features can also be updated, either by directly taking the results of ϕ_m or by using another
 929 message function ϕ_e .

930 Message passing is a very generic way of describing the process of GNN and it can be specialized
 931 for convolutional filtering [49], diffusion [63] and many other specific operation. GNN are used in a
 932 wide variety of application such as regression problematics, node classification, edge classification,
 933 node and edge prediction, ...

934 It is a very versatile but complex tool.

935 3.2.4 Adversarial Neural Network (ANN)

936 The adversarial machine learning, Adversarial Neural Networks (ANN) in the case of neural net-
 937 work, is a family of unsupervised machine learning algorithms where the learning algorithm (gen-
 938 erator) is competing against another algorithm (discriminator). Taking the example of Generative
 939 Adversarial Networks, concept initially developed by Goodfellow et al. [64], the discriminator goal
 940 is to discriminate between data coming from a reference dataset and data produced by the generator.
 941 The generator goal, on the other hand, is to produce data that the discriminator would not be able to
 942 differentiate from data from the reference dataset. The expression of duality between the two models
 943 is represented in the loss where, at least a part of it, is driven by the results of the discriminator.

944 3.2.5 Training procedure

945 A neural network without the adequate training is like an empty shell. If the parameters are not
 946 optimized they are, most of the time, initialized to random number and so the output will just be
 947 random. The training is a key step in the production of a solid and reliable NN. This section aim to
 948 give an overview of the different concept and tools used in the training of our neural networks.

949 Training lifecycle

950 The training of NN does not follow strict rules, you could imagine totally different lifecycle but I will
 951 describe here the one used in this thesis, the most common one.

952 The training is split into *epochs* during which the NN will train on a set of subsamples called *batch*.
 953 The size of those batch is called *batch size*, a.k.a. the number of data it contains (how many images,
 954 how many events,...). Each process of a batch is called a *step*. At the end of each epochs, the neural
 955 network is evaluated over a validation dataset. This validation dataset is not used for training (no
 956 gradient of the loss is computed) and is used as reference for the network performance and monitor
 957 overtraining (see section 3.2.6). Most of the time, the parameters are updated at each step using the
 958 mean loss over the batch and the optimizer hyperparameters are updated at each epochs.

959 **The optimizer**

960 As briefly introduced section 3.2, the parameters of the neural network are optimized using the
 961 gradient descent method. We calculate the gradient of the mean loss over the batch with respect
 962 of each parameters and we update the parameters in accord to minimize the loss. The gradient is
 963 computed backward from the loss up to the first layer parameters using the chain rule:

$$\frac{\partial \mathcal{L}}{\partial \theta_1} = \frac{\partial \theta_2}{\partial \theta_1} \frac{\partial \mathcal{L}}{\partial \theta_2} = \frac{\partial \theta_2}{\partial \theta_1} \frac{\partial \theta_3}{\partial \theta_2} \frac{\partial \mathcal{L}}{\partial \theta_3} = \frac{\partial \theta_2}{\partial \theta_1} \prod_{i=2}^{N-1} \frac{\partial \theta_{i+1}}{\partial \theta_i} \frac{\partial \mathcal{L}}{\partial \theta_N} \quad (3.9)$$

964 where θ is a parameter, i is the layer index. We see here that the gradient of the first layer is dependent
 965 of the gradient of all the following layers. We thus need to compute the gradient closest to loss first
 966 before computing the gradient of the earlier layers. This is called the *backward propagation*.

967 This update of the parameters is done following an optimizer policy. Those optimizers depends on
 968 hyperparameters. The ones used in this thesis are:

- 969 1. SGD (Stochastic Gradient Descent). This is the simplest optimizer, it depend on only one
 970 hyperparameter, the learning rate λ (LR) and update the parameters θ following

$$\theta_{t+1} = \theta_t - \lambda \frac{\partial \mathcal{L}}{\partial \theta} \Big|_{\theta_t} \quad (3.10)$$

971 where t is the step index. It is a powerful optimizer but is very sensible to local minima of the
 972 loss in the parameters phase space as illustrated in figure 3.5a.

- 973 2. Adam [55]. The concept is, in short, to have and SGD but with momentum. Adam possess
 974 two momentum $m(\beta_1)$ and $v(\beta_2)$ which are respectively proportional to $\frac{\partial \mathcal{L}}{\partial \theta}$ and $(\frac{\partial \mathcal{L}}{\partial \theta})^2$. β_1
 975 and β_2 are hyperparameters that dictate the moment update at each optimization step. The
 976 parameters are then upgraded following

$$m_{t+1} = \beta_1 m_t + (1 - \beta_1) \frac{\partial \mathcal{L}}{\partial \theta} \quad (3.11)$$

$$v_{t+1} = \beta_2 v_t + (1 - \beta_2) \left(\frac{\partial \mathcal{L}}{\partial \theta} \right)^2 \quad (3.12)$$

$$\theta_{t+1} = \theta_t - \lambda \frac{m_{t+1}}{\sqrt{v_{t+1}} + \epsilon} \quad (3.13)$$

977 where ϵ is a small number to prevent divergence when v is close to 0. These momentums
 978 allow to overcome small local minima in the parameters phase space as illustrated in figure
 979 3.5a.

980 The LR is a crucial parameter in the training of NN, as illustrated in figure 3.6. To prevent possible
 981 issues, we setup scheduler policies.

982 **Scheduler policies**

983 Sometimes we want to update our hyperparameters or take a set of action during the training
 984 procedure. We use for this scheduler policies, for example a common policy is a decrease of the
 985 learning rate after each epochs. The reasoning is that if the learning rate is too high, the optimizer
 986 will continuously miss the minimum and oscillate around it (figure 3.6a). By reducing the learning
 987 rate, we allow it to make more fine steps in the parameters phase space, hopefully converging to the
 988 true minima.

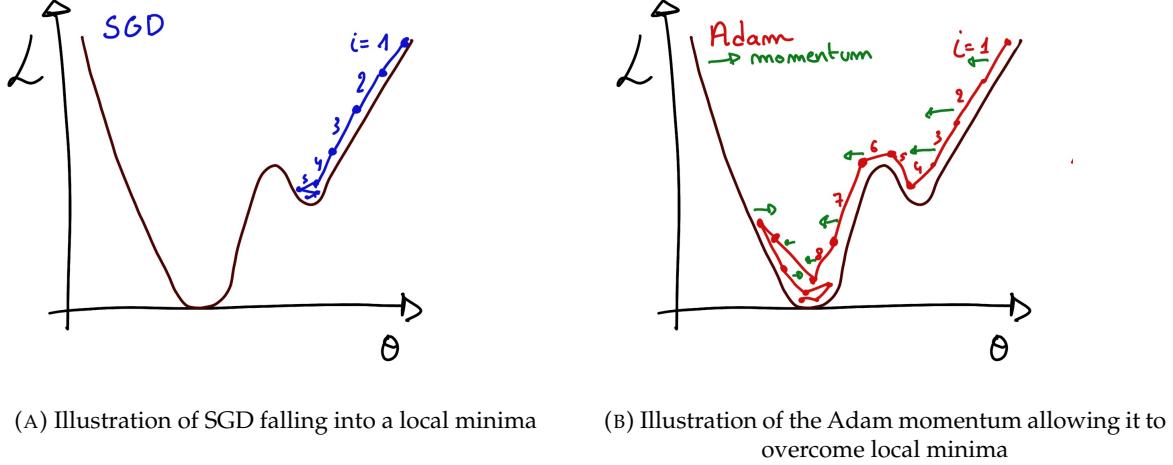


FIGURE 3.5

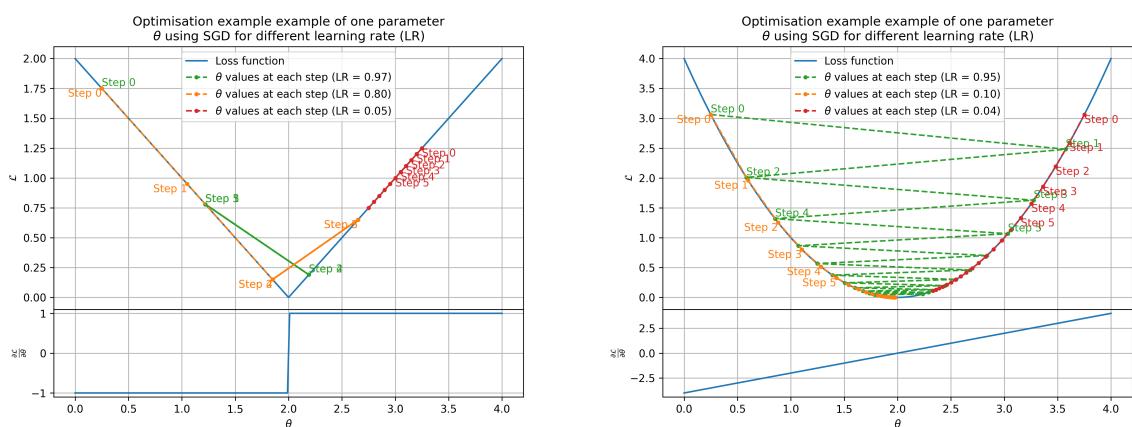
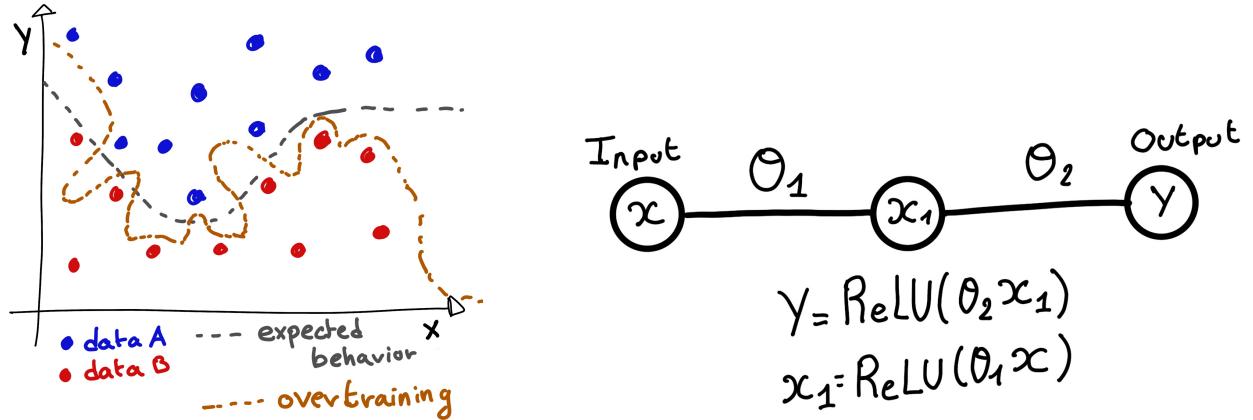
(A) Illustration of the SGD optimizer on one parameter θ on the MAE Loss. We see here that it has trouble reaching the minima due to the gradient being constant.(B) Illustration of the SGD optimizer on one parameter θ on the MAE Loss. We see two different behavior: A smooth one (orange and red) when the LR is small enough and a more chaotic one when the LR is too high.

FIGURE 3.6 – Illustration of the SGD optimizer. In blue is the value of the loss function, orange, green and red are the path taken by the optimized parameter during the training for different LR.



(A) Illustration of overtraining. The task at hand is to determine depending on two input variable x and y if the data belong to the dataset A or the dataset B . The expected boundary between the two dataset is represented in grey. A possible boundary learnt by overtraining is represented in brown.

(B) Illustration of a very simple NN

FIGURE 3.7

985 Another policy that is often used is the save of the best model. In some situations, the loss value after
 986 each epoch will strongly oscillate or even worsen. This policy allows us to keep the best version
 987 of the model attained during the training phase.

988 3.2.6 Potential pitfalls

989 Apart from being stuck in local minima, there are also other behaviors and effects we want to prevent
 990 during training.

991 Overtraining

992 This happens when the network learns the specificities of the training dataset instead of a more general
 993 representation of the underlying data distribution. This can happen if there is not enough data
 994 in comparison to the number of learning parameters, if the data contains some specific signatures
 995 specific to the training dataset or if it trains for too long on the same dataset. This behavior is illustrated
 996 in figure 3.7a. Overtraining can be fought in multiple ways, for example:

- 997 — **More data.** By having more data in the training dataset, the network will not be able to learn the
 998 specificities of every data.
- 999 — **Less parameters.** By reducing the number of parameters, we reduce the computing and
 1000 learning capacities of the network. This will force it to fallback to generalist behaviors.
- 1001 — **Dropout.** This technique implies to randomly set part of the neural network to 0. By doing
 1002 this, we force the redundancy in its computing capability and, in a way, modify the data
 1003 decreasing the possibility for specific learning.
- 1004 — **Early stopping.** During the training we monitor the network performance over a validation
 1005 dataset. The network does not train on this dataset and thus cannot learn its specificities. If
 1006 the loss on the training dataset diverges too much from the loss on the validation dataset, we
 1007 can stop the training earlier to prevent it from overtraining.

1008 **Gradient vanishing**

1009 Gradient vanishing is the effect of the gradient being so small for the upper layer that the parameters
 1010 are barely updated after each step. This cause the network to be unable to converge to the minima.

1011 This comes from the way the gradient descent is calculated. Imagine a simple network composed of
 1012 three fully connected layers: the input layer, a intermediate layer and the output layer. Let L be the
 1013 loss, θ_1 the parameter between the input and the intermediate layer and θ_2 the parameter between
 1014 the intermediate and output layer. This network is schematized in figure 3.7b.

1015 The gradient for θ_1 will be computed using the chain rule presented in equation 3.9. Because θ_1
 1016 depends on θ_2 , if the gradient of θ_2 is small, so will be the gradient of θ_1 . Now if we would have
 1017 much more layer, we can see how the subsequent multiplication of small gradients would lead to
 1018 very small update of the parameters thus "vanishing gradient".

1019 Multiple actions can be taken to prevent this effect such as:

- 1020 — **Batch normalization:** In this case we apply a normalization layer that will normalize the data
 1021 so that, let D be the data, $\langle D \rangle = 0$ and $\sigma_D = 1$. This help the weight of the network to
 1022 maintain an appropriate scale.
- 1023 — **Residual Network (ResNet) [65]:** Residual network is a technique for neural network in
 1024 which, instead of just sequentially feeding the results of each layer to the next one, you ask
 1025 each layer to calculate the residual of the input data. This technique is illustrated in figure 3.8.

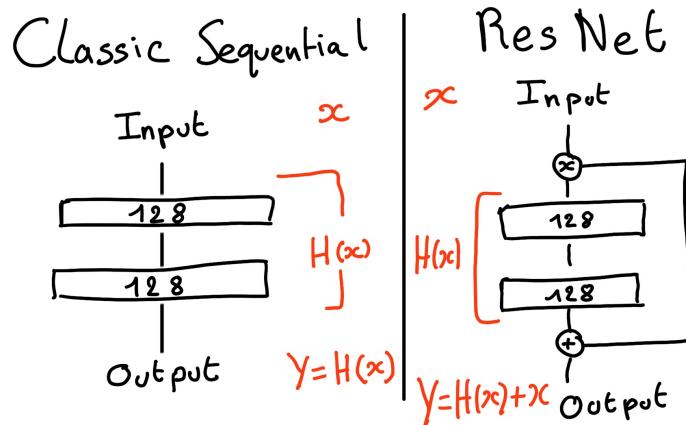


FIGURE 3.8 – Illustration of the ResNet framework

1026 **Gradient explosion**

Gradient explosion happens when the consecutive multiplication of gradient cause exponential grow in the parameter value or if the training lead the network in part of the parameter space where the gradient is significantly higher than usual. For illustration, consider that the loss dependency in θ follow

$$\mathcal{L}(\theta) = \frac{\theta^2}{2} + e^{4\theta}$$

$$\frac{\partial \mathcal{L}}{\partial \theta} = \theta + 4e^{4\theta}$$

1027 The explosion is illustrated in figure 3.9 where we can see that the loss degrade with each step of
 1028 optimization. In this illustration it is clear that reducing the learning rate suffice but this behaviour
 1029 can happens in the middle of the training where the learning rate schedule does not permit reactivity.

1030 There exist solutions to prevent this explosions:

- 1031 — **Gradient clipping:** In this case we work on the gradient so that the norm of gradient vector
 1032 does not exceed a certain threshold. In our illustration in figure 3.9 the gradient for $\theta > 0$
 1033 could be clipped at 3 for example.
- 1034 — **Batch normalization:** For the same reasons as for gradient vanishing, normalizing the input
 1035 data help reduce erratic behaviour.

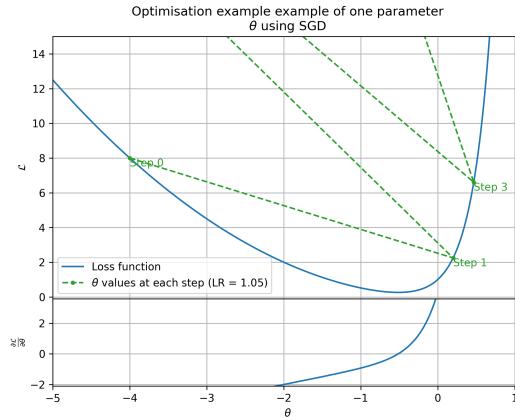


FIGURE 3.9 – Illustration of the gradient explosion. Here it can be solved with a lower learning rate but its not always the case.

¹⁰³⁶ **Chapter 4**

¹⁰³⁷ **Image recognition for IBD
reconstruction with the SPMT system**

Dave - Give me the position and momentum, HAL.

HAL - I'm afraid I can't do that Dave.

Dave - What's the problem ?

HAL - I think you know what the problem is just as well as I do.

Dave - What are you talking about, HAL?

HAL - $\sigma_x \sigma_p \geq \frac{\hbar}{2}$

¹⁰⁴⁰ As explained in chapter 2, JUNO is an experiment composed of two systems, the Large Photomultiplier (LPMT) system and the Small Photomultiplier (SPMT) system. Both of them observe the same ¹⁰⁴¹ physics events inside of the same medium but they differ in their photo-coverage, respectively 75.2% ¹⁰⁴² and 2.7%, their dynamic range (see section 2.2.2), a thousands versus a few dozen, and their front-end ¹⁰⁴³ electronics (see section 2.2.2).

¹⁰⁴⁵ They are complementary in their strengths and weaknesses and support each other, this is what ¹⁰⁴⁶ we call *Dual Calorimetry*. One important point is their differences in expected resolution, the LPMT ¹⁰⁴⁷ system outperform largely the SPMT system but is subject to effects such as charge non linearity [29] ¹⁰⁴⁸ that could bias the reconstruction. Effects that the SPMT system is impervious to. This topic will ¹⁰⁴⁹ be studied in more detail in chapter 7. Also, due to the dynamic range of the LPMT, in case of high ¹⁰⁵⁰ energy and high density event such as core-collapse supernova, the LPMT system could saturate and ¹⁰⁵¹ the lower photo-coverage become a benefit.

¹⁰⁵² Thus, although event reconstruction algorithm and physics analysis combines both LPMT and SPMT ¹⁰⁵³ systems, individual approach are key studies to understand the detector and ensure their reliability. ¹⁰⁵⁴ This topic will also be studied in more details in chapter 7. The subject of this chapter is to propose ¹⁰⁵⁵ a machine learning algorithm for the SPMT reconstruction based on Convolutional Neural Network ¹⁰⁵⁶ (CNN).

¹⁰⁵⁷ **4.1 Motivations**

¹⁰⁵⁸ As explained in chapter 3, Machine Learning (ML) algorithms shine when modeling highly dimensional ¹⁰⁵⁹ data from a given dataset. In our case, we have access to complete monte-carlo simulation of ¹⁰⁶⁰ our detector to produce arbitrary large datasets that could represent multiple years of data taking. ¹⁰⁶¹ Ideally ML algorithms would be able to consider the entirety of the information in the detector and ¹⁰⁶² converge on the best parameters to yield optimal results, while classical methods could be biased by ¹⁰⁶³ the prior knowledge of the detector and physics processes. To study this potential phenomena, we

1064 will compare our machine algorithm to a classical reconstruction method developed for energy and
 1065 vertex reconstruction [66].

1066 We have access to a very detailed simulation of the detector (section 2.5) that will allow us to simulate
 1067 arbitrary large dataset while giving access to all the physics parameters of the event. Those
 1068 parameters include the target of our reconstruction algorithms: the vertex and energy of our event.
 1069 As introduced above, we hope that the ML algorithm will be able to use all the informations in the
 1070 event, but that could lead that potential mismodelings in our simulation could be exploited by the
 1071 algorithm. This specific subject will be studied in chapter 6.

1072 4.2 Method and model

1073 One of simplest way to look at JUNO data is to consider the detector as an array of geometrically
 1074 distributed sensors on a sphere. Their repartition is almost homogeneous, on this sphere surface
 1075 providing an almost equal amount of information per unit surface on this sphere. It is then tempting
 1076 to represent the detector as a spherical image with the PMTs in place of pixels. Two events with two
 1077 different energy or position would produce two different images.

1078 The most common approach in machine learning for image processing and image recognition is the
 1079 Convolutional Neural Network (CNN). It is widely used in research and industry [57, 67–69] due to
 1080 its strengths (see section 3.2.2) and has proven its relevance in image processing.

1081 Some CNN are developed to process spherical images [70] but for the sake of simplicity and as a
 1082 first approach we decided to go with a planar projection of the detector, approach that has proven its
 1083 efficiency using the LPMT system (see section 2.6.3). The details about this planar projection will be
 1084 discussed in section 4.2.2.

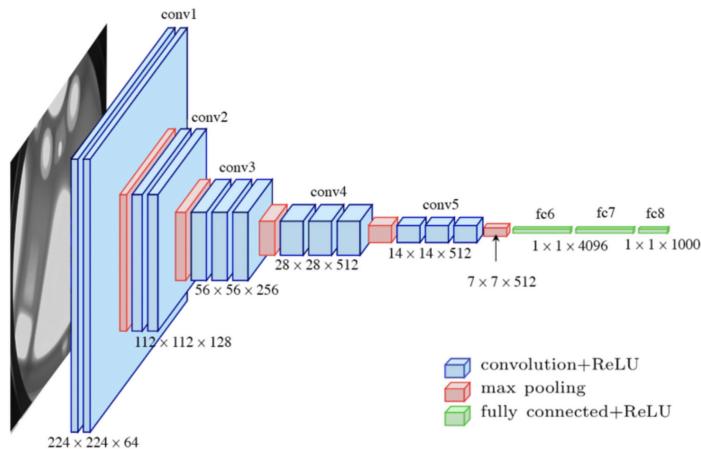


FIGURE 4.1 – Graphic representation of the VGG-16 architecture, presenting the different kind of layer composing the architecture.

1085 4.2.1 Model

1086 The architecture we use is derived from the VGG-16 architecture [57] illustrated in figure 4.1. We
 1087 define a set of hyperparameters that will define the size, complexity and computational power of the
 1088 NN. The chosen hyperparameters are detailed below and their values are presented in table 4.1.

- 1089 — **N_{blocks}**: the number of convolution blocks, a block being composed of two convolutional
1090 layers with 3×3 filters using ReLU activation function, a 3×3 max-pooling layer (except for
1091 the last block).
- 1092 — **N_{channels}**: The number of channels in the first block. The number of channels in the subse-
1093 quent blocks is computed using $N_{\text{channels}}^i = i * N_{\text{channels}}$, $i \in [1..N_{\text{blocks}}]$.
- 1094 — **FCDNN configuration**: The result of the last convolution layer is flattened then fed to a
1095 FCDNN. Its configuration is expressed as a sequence of fully connected linear layer using
1096 the PReLU activation function. For example $2 * 1024 + 2 * 512$ is the sequence of 2 layers
1097 with a width of 1024 followed by 2 other layers with a width of 512. Finally the last layer
1098 is a 4 neurons wide linear layers without activation function. Each neurons of the last layer
1099 represent a component of the interaction vertex: Energy, X, Y, Z.
- 1100 — **Loss**: The loss function. In this work we study two different loss function ($E + V$) and ($E_r +$
1101 V_r) detailed below.

$$(E + V)(E, x, y, z) = \left\langle (E - E_{\text{true}})^2 + 0.85 \sum_{\lambda \in [x, y, z]} (\lambda - \lambda_{\text{true}})^2 \right\rangle \quad (4.1)$$

$$(E_r + V_r)(E, x, y, z) = \left\langle \frac{(E - E_{\text{true}})^2}{E_{\text{true}}} + \frac{10}{R} \sum_{\lambda \in [x, y, z]} (\lambda - \lambda_{\text{true}})^2 \right\rangle \quad (4.2)$$

1102 where R is the radius of the CD. With the energy in MeV and the distance in meters, we use the factor
1103 0.85 and 10 to equilibrate the two term of the loss function so they have the same magnitude.

- 1104 — The loss function ($E + V$) is close to a simple Mean Squared Error (MSE). MSE is one of the
1105 most basic loss function, the derivative is simple and continuous in every point. It is a strong
1106 starting point to explore the possibility of CNNs.
- 1107 — $(E_r + V_r)$ can be seen as a relative MSE.

1108 The idea is that: due to the inherent statistic uncertainty over the number of collected Number of
1109 Photo Electrons (NPE), the absolute resolution $\sigma(E - E_{\text{true}})$ will be larger at higher energy than at
1110 low energy. But we expect the *relative* energy resolution $\frac{\sigma(E - E_{\text{true}})}{E_{\text{true}}}$ to be smaller at high energy than
1111 lower energy as illustrated in figure 2.22. Because of this, by using simple MSE the most important
1112 part in the loss come from the high energy part of the dataset whereas with a relative MSE, the
1113 most important part become the low energy events in the dataset. We hope that by using a relative
1114 MSE, the neural network will focus on low energy events where the reconstruction is considered the
1115 hardest.

1116 Each combination of those hyperparameters (for example ($N_{\text{blocks}} = 2, N_{\text{channels}} = 32$, FCDNN =
1117 $(2 * 1024)$, Loss = $(E + V)$)), subsequently designated as configurations, is then tested and compared
1118 to each other over an analysis sample.

1119 On top those generated models, we define 4 hand tailored models:

- 1120 — “gen_0”: $N_{\text{blocks}} = 4, N_{\text{channels}} = 64$, FCDNN configuration: $1024 * 2 + 512 * 2$, Loss := $E + V$
- 1121 — “gen_1”: $N_{\text{blocks}} = 4, N_{\text{channels}} = 64$, FCDNN configuration: $1024 * 2 + 512 * 2$, Loss := $E_r + V_r$
- 1122 — “gen_2”: $N_{\text{blocks}} = 5, N_{\text{channels}} = 64$, FCDNN configuration: $4096 * 2 + 1024 * 2$, Loss := $E + V$
- 1123 — “gen_3”: $N_{\text{blocks}} = 5, N_{\text{channels}} = 64$, FCDNN configuration: $4096 * 2 + 1024 * 2$, Loss := $E_r + V_r$

1124 We cannot use the mean loss because we consider multiple loss functions, there is no guarantee that
1125 comparison of their numerical value will be meaningful. We use multiple observables to rank the
1126 performances of each configuration:

- 1127 — The mean absolute energy error $\langle E \rangle = \langle |E - E_{\text{true}}| \rangle$. It is an indicator of the energy bias of our
1128 reconstruction.
- 1129 — The standard deviation of the energy error $\sigma E = \sigma(E - E_{\text{true}})$. This the indicator on our
1130 precision in energy reconstruction.
- 1131 — The mean distance between the reconstructed vertex and the true vertex $\langle V \rangle = \langle |\vec{V} - \vec{V}_{\text{true}}| \rangle$.
1132 This an indicator of the bias and precision of our vertex reconstruction.

N_{blocks}	{2, 3, 4}
$N_{channels}$	{32, 64, 128}
FCDNN configurations	2 * 1024 2 * 2048 + 2 * 1024 3 * 2048 + 3 * 512 2 * 4096
Loss	{ $E + V, E_r + V_r$ }

TABLE 4.1 – Sets of hyperparameters values considered in this study

— The standard deviation of the distance between the true and reconstructed vertex $\sigma V = \sigma |\vec{V} - \vec{V}_{true}|$. This is an indicator if the precision in our vertex reconstruction.

The models were developped in Python using the pytorch framework [59] using NVIDIA A100 [71] and NVIDIA V100 [72] gpus. The A100 was split in two, thus the accessible gpu memory was 20 Gb making it impossible to train some of the architectures due to memory consumption.

The training was monitored in realtime by a custom tooling that was developed during this thesis, DataMo [73].

The training of one model takes between 4h and 15h depending of its size, overall training the full 72 model takes around 500 GPU hours. Even with parallel training, this random search hyper-optimisation was time consuming.

4.2.2 Data representation

This data is represented as 240×240 images with a charge Q channel and a time t channel. The SPMTs are then projected on the plane as illustrated in figure 4.2. The x position is proportional to θ and the y position is defined by $\phi \sin \theta$ in spherical coordinates. $\theta = 0$ is defined as being the top of the detector and $\phi = 0$ is defined as an arbitrary direction in the detector. In practice, $\phi = 0$ is given by the MC simulation.

$$x = \left\lfloor \frac{\theta \cdot H}{\pi} \right\rfloor, \theta \in [0, \pi] \quad (4.3)$$

$$y = \left\lfloor \frac{(\phi + \pi) \sin \theta \cdot W}{2\pi} \right\rfloor, \phi \in [-\pi, \pi], \theta \in [0, \pi] \quad (4.4)$$

where H is the height of the image, W the width of the image and $(0, 0)$ the top left corner of the image.

When two SPMTs are in the same pixel, the charges are summed and the lowest of the hit-time is chosen. The SPMTs being located close to each other, we expect the time difference between two successive physics signals, two photons being collected, to be small. The first hit time is chosen because it can be considered as the relative propagation time of the photons that went the "straightest", i.e. that went under the less perturbation of the two. The only potential problem in using this first time come from the Dark Noise (DN). Its time distribution is uniform over the signal and could come before a physics signal on the other SPMT in the pixel. In that case, the time information in the pixel become irrelevant and we lose the timing information for this part of the detector. As illustrated in figure 4.2 the image dimension have been optimized so that at most two SPMTs are in the same pixel while keeping the number of empty pixels relatively low to prevent this kind of issue.

While it could be possible to use larger images (more pixel) to prevent overlapping, keeping image small images gives multiple advantages:

- 1163 — As presented in section 4.2.1, the convolution filter we use are 3×3 convolution filter, meaning
1164 that if SPMTs would be separated by more than one pixel, the first filter would only see one
1165 SPMT per filter. This behavior would be kind of counterproductive as the first convolution
1166 block would basically be a transmission layer and would just induce noise in the data.
- 1167 — It keep the network relatively small, while this do not impact the convolution layers, the
1168 flatten operation just before the FCDNN make the number parameters in the first layer of
1169 it dependent on the size of the image.
- 1170 — It reduce the number of empty pixel in the image.

1171 The question of empty pixel is an important question in this data representation. There is two kind
1172 of empty pixels in the data.

1173 The first kind is pixel that contain a SPMT but the SPMT did not get hit nor registered any dark noise
1174 during the event. In this case, the charge channel is zero, which have a physical meaning but then
1175 come the question of the time layer. One could argue that the correct time would be infinity (or the
1176 largest number our memory allows us) because the hit “never” happened, so extremely far from the
1177 time of the event. This cause numerical problem as large number, in the linear operation that are
1178 happening in the convolution layers, are more significant than smaller value. We could try to encode
1179 this feature in another way but no number have any significance due to our time being relative to
1180 the trigger of the experiment so -1 for example is out of question. Float and Double gives us access
1181 to special value such as NaN (Not a Number) [74] but the behavior is to propagate the NaN which
1182 leaves us with NaN for energy and position. We choose to keep the value 0 because it’s the absorbing
1183 element of multiplication, absorbing the “information” of the parameter it would be multiplied by.
1184 It also can be though as no activation in the ReLU activation function.

1185 The second kind of pixel is pixel that do not represent parts of the detector such as the corners of
1186 the image. The question is basically the same, what to put in the charge and the time channel. The
1187 decision is to set the charge and time to 0 following the above reasoning. It’s important to keep in
1188 mind the fact that a part of the detector that has not been hit is also an information: There is no signal
1189 in this part of the detector. This problematic will be explored in more details in chapter 5.

1190 Another problematic that happens with this representation, and this is not dependent of the chosen
1191 projection, is the deformation in the edges of the image and the loss of the neighbouring information
1192 in the for the SPMTs at the edge of the image $\phi \sim 180^\circ$. This deformation and neighbouring loss
1193 could be partially circumvented as explained in section 4.5

1194 4.2.3 Dataset

1195 In this study we will discuss two datasets of one millions events:

- 1196 — **J21:** The first one comes from the JUNO official mc simulation J21v1r0-Pre2 (released the 18th
1197 August 2021). This historical version is the one on which the classical algorithm presented in
1198 [66] was developed. This dataset is used as a reference for comparison to classical algorithm.
1199 The data in this dataset is *detsim* level (see section 2.5), where only the physic is simulated.
1200 The charge and time biases and uncertainties are implemented using toy MC adjusted using
1201 [26, 75]. The time window is not based on a selection algorithm but $t_0 := t = 0$ is defined as
1202 the first PMT hit. The window goes up to $t_0 + 1000$ ns.
- 1203 — **J23:** The second comes from the JUNO official monte-carlo simulations J23.0.1-rc8.dc1 (re-
1204 leased the 7th January 2024). The data is *calib* level (see section 2.5). Here the charge comes
1205 from the waveform integration, the time window resolution and trigger decision are all simu-
1206 lated inside the software. This dataset is more realistic and is used to confirm the performance
1207 of our algorithm.

1208 To put in perspective this amount of data, the expected IBD rate in JUNO is 47 / days. Taking into
1209 account the calibration time, and the source reactor shutdown, it amount to $\sim 94'000$ IBD events
1210 in 6 years. With this million of event, we are training the equivalent of ~ 10 years of data. With

1211 this amount we reach a density of $4783 \frac{\text{event}}{\text{m}^3 \cdot \text{MeV}}$, meaning our dataset is representative of the multiple
 1212 event scenarios that could be happening in the detector.

1213 While we expect and hope the monte-carlo simulation to give use a realistic representation of the detector,
 1214 there could be effect, even after the fine-tuning on calibration data, that the simulation
 1215 cannot handle. Thus, once the calibration will be available, we will need to evaluate, and if needed
 1216 retrain, the network on calibration data to establish definitive performances.

1217 The simulated data is composed of positron events, uniformly distributed in the CD volume and in
 1218 kinetic energy over $E_k \in [0; 9]$ MeV producing a deposited energy $E_{dep} \in [1.022; 10.022]$ MeV. This is
 1219 done to mimic the signal produced by the IBD prompt signal. Uniform distributions are used so that
 1220 the CNN does not learn a potential energy distribution, favoring some part of the energy spectrum
 1221 instead of other.

1222 Those events can be considered as “optimistic” as there is no pile-up with potential background or
 1223 other IBD.

1224 4.2.4 Data characteristics

1225 To delve a bit into the kind of data we will use, you can find in figure 4.2 the repartition of the SPMTs
 1226 in the image. The color represent the number of SPMTs per pixel.

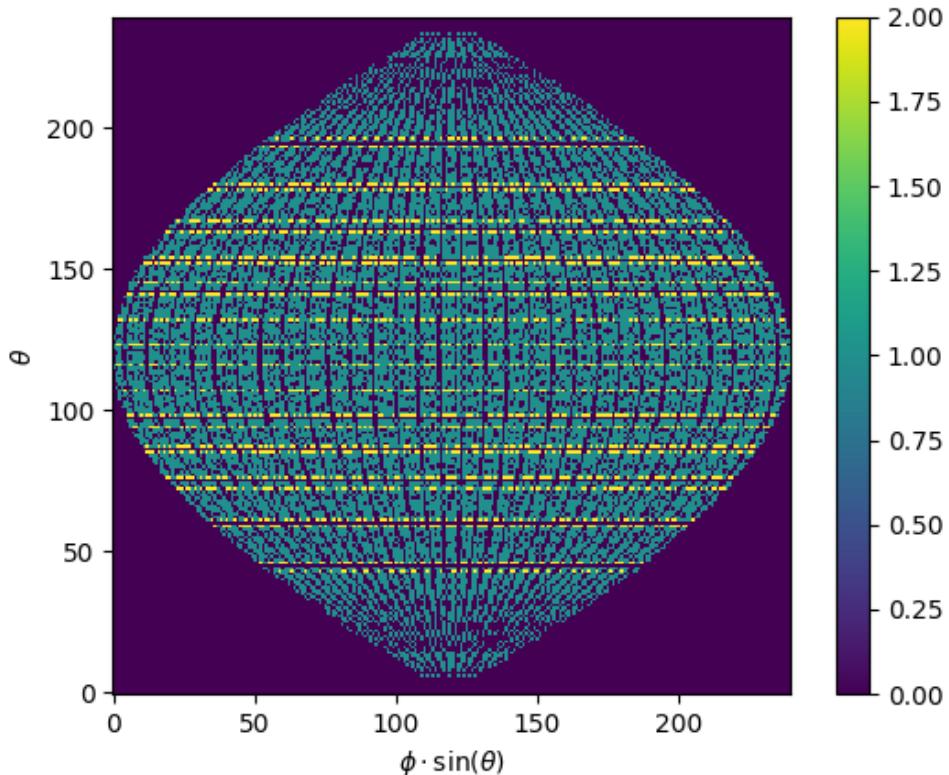


FIGURE 4.2 – Repartition of SPMTs in the image projection. The color scale is the number of SPMTs per pixel

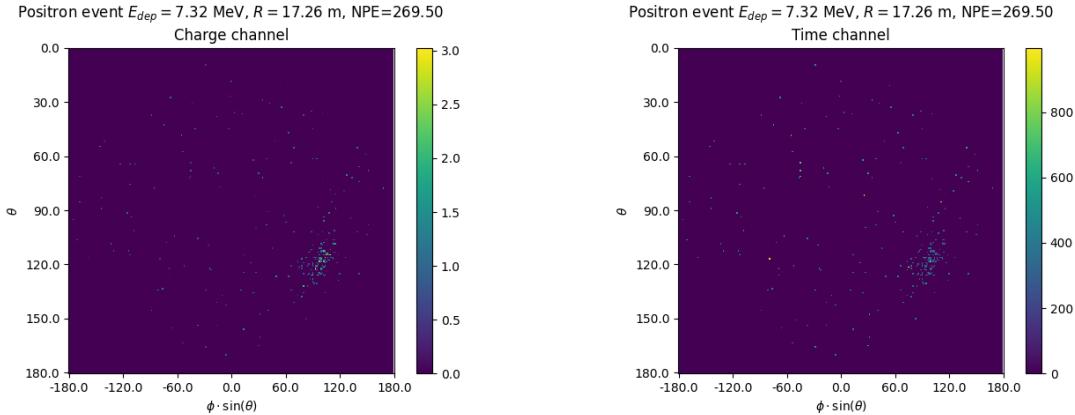


FIGURE 4.3 – Example of a high energy, radial event. We see a concentration of the charge on the bottom right of the image, clear indication of a high radius event. **On the left:** the charge channel. The color is the charge in each pixel in NPE equivalent. **On the right:** The time channel in nanoseconds.

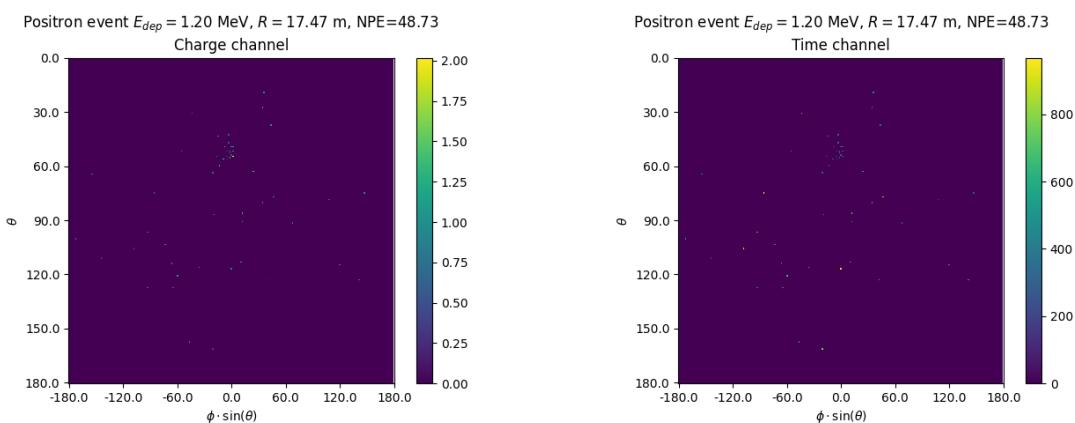


FIGURE 4.4 – Example of a low energy, radial event. The signal here is way less explicit, we can kind of guess that the event is located in the top middle of the image. **On the left:** the charge channel. The color is the charge in each pixel in NPE equivalent. **On the right:** The time channel in nanoseconds.

1227 In figures 4.3, 4.4, 4.5 and 4.6 are presented events from J23 for different positions and energies.
1228 We see some characteristics and we can instinctively understand how the CNN could discriminate
1229 different situations.

To give an idea of the strength of the signal in comparison to the dark noise background, figure 4.7a present the distribution of the ratio of NPE per deposited energy. Assuming a linear response of the LS we can model:

$$NPE_{tot} = E_{dep} \cdot P_{mev} + D_N \quad (4.5)$$

$$\frac{NPE_{tot}}{E_{dep}} = P_{mev} + \frac{D_N}{E_{dep}} \quad (4.6)$$

1230 where NPE_{tot} is the total number of PE detected by the event, P_{mev} is the mean number of PE detected
1231 per MeV and D_N is the dark noise contribution that is considered energy independent. In the case
1232 where the readout time window is dependent of the energy the dark noise contribution become

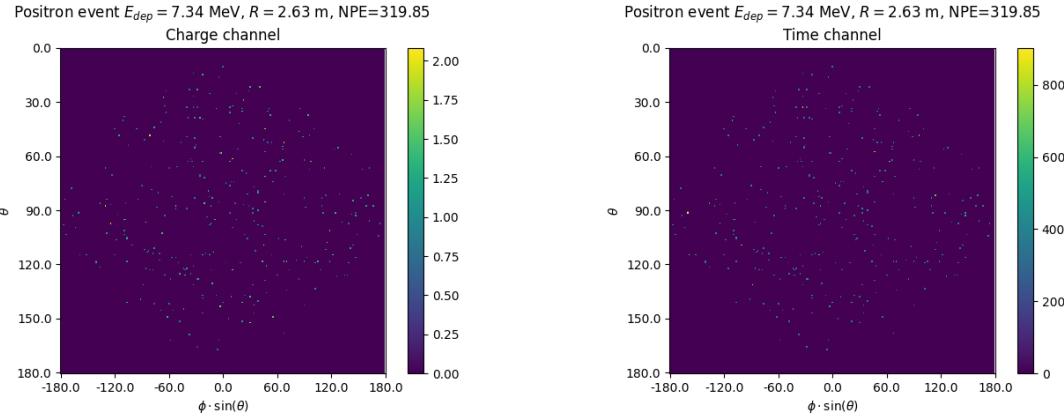


FIGURE 4.5 – Example of a high energy, central event. In this image we can see a lot of signal but uniformly spread, this is indicative of a central event. **On the left:** the charge channel. The color is the charge in each pixel in NPE equivalent. **On the right:** The time channel in nanoseconds.

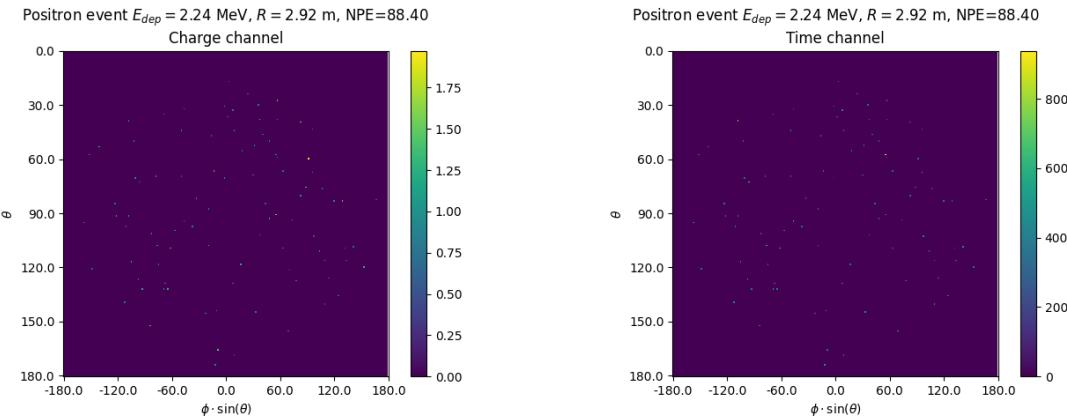
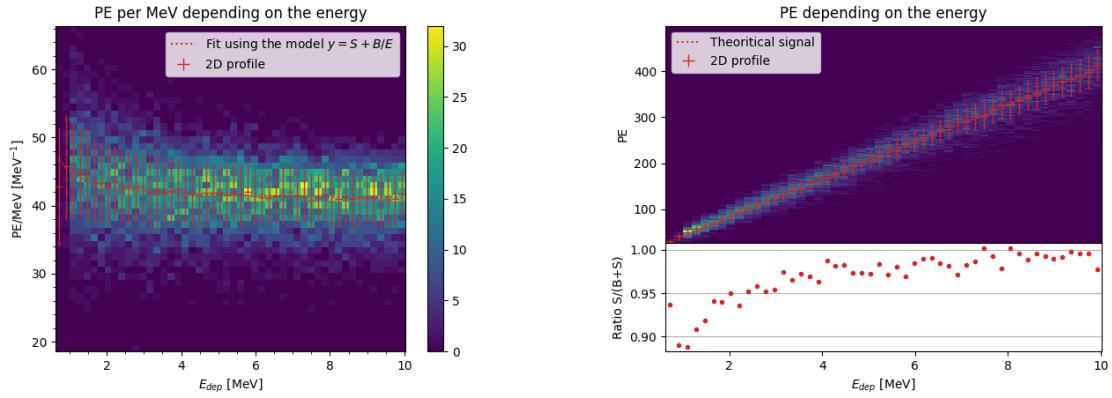


FIGURE 4.6 – Example of a low energy, central event. Here there is no clear signal, the uniformity of the distribution should make it central. **On the left:** the charge channel. The color is the charge in each pixel in NPE equivalent. **On the right:** The time channel in nanoseconds.

¹²³³ energy dependant, also the LS response is realistically energy dependant but figure 4.7a shows that
¹²³⁴ we have heavily dominated by statistical uncertainties which is why we are using this simple model.
¹²³⁵ The fit shows a light yield of 40.78 PE/MeV and a dark noise contribution of 4.29 NPE. As shown in
¹²³⁶ figure 4.7b, the physics makes for 90% of the signal at low energy.

¹²³⁷ 4.3 Training

¹²³⁸ The optimizer used for the training is the Adam [55] optimizer, with a learning rate λ of 1e-3. The
¹²³⁹ other hyperparameters were left to their default value ($\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 1e - 8$). The
¹²⁴⁰ learning rate was reduced exponentially during the training at a rate of $\gamma = 0.95$, thus $\lambda_{i+1} = 0.95\lambda_i$
¹²⁴¹ where i is the epoch.
¹²⁴² The training was composed of 30 epochs, each epoch constituted of 10k steps using a batch size of 64



(A) Distribution of PE/MeV in the J23 Dataset. This distribution is profiled and fitted using equation 4.6

(B) On top: Distribution of PE vs Energy. On bottom: Using the values extracted in 4.7a, we calculate the ration signal over background + signal

FIGURE 4.7

1243 events. The validation was computed over a 100 steps on the validation dataset.

1244 4.4 Results

1245 Before presenting the results, lets discuss the different observables.

1246 The event are considered point like in this study. The target truth position, or vertex, is the mean po-
1247 sition of the energy deposits of the positron and the two annihilation gammas. Due to the symmetries
1248 of the detector, we mainly consider and discuss the bias and precision evolution depending of the
1249 radius R but we will still monitor the performances depending of the spheric angle θ and ϕ . From the
1250 detector construction and effect we expect dependency in radius due to the TR area effect presented
1251 in section 2.6 and the possibility for the positron or the gammas to escape from the CD for near the
1252 edge events. We also expect dependency in θ , the top of the experiment being non-instrumented due
1253 to the filling chimney. It is also to be noted that the events in the dataset are uniformly distributed in
1254 the CD, and so are uniformly distributed in R^3 and ϕ . The θ distribution is not uniform and we will
1255 have more event for $\theta \sim 90^\circ$ than $\theta \sim 0^\circ$ or $\theta \sim 180^\circ$.

1256 We define multiple energy in JUNO:

- 1257 — E_ν : The energy of the neutrino.
- 1258 — E_k : The kinetic energy of the resulting positron from the IBD.
- 1259 — E_{dep} : The deposited energy of the positron and the two annihilation gammas.
- 1260 — E_{vis} : The equivalent visible energy, so E_{dep} after the detector effect such as the absorption of
scintillation photons by the LS and the LS response non-linearity.
- 1261 — E_{rec} : The reconstructed energy by the reconstruction algorithm. The expected value depend
on the algorithm we discuss about. For example the algorithm presented in section 2.6 is
reconstructing E_{vis} while the ones presented in section 2.6.3 reconstruct E_{dep} .

1262 In this study, we will set E_{dep} as our target for energy reconstruction. This choice is motivated by the
1263 ease with which we can retrieve this information in the monte-carlo data while E_{vis} is less trivial to
1264 retrieve.

1268 **4.4.1 J21 results**

1269 Those results comes from the “gen_30” model, meaning then 30th model generated using the table
 1270 [4.1](#) or
 1271 — “gen_30”: $N_{blocks} = 3$, $N_{channels} = 32$, FCDNN configuration: $2048 * 2 + 1024 * 2$, Loss := $E + V$
 1272 The performances of its reconstruction are presented in blue in figure [4.8](#). Superimposed in black is
 1273 the performances of the classical algorithm from [66].

1274 **Energy reconstruction**

1275 By looking at the figure [4.8a](#) and [4.8b](#), the CNN has similar performances in its energy resolution.
 1276 Only at the end of the energy range does the resolution get a little better.

1277 This is explained by looking at the true and reconstructed energy distributions in figure [4.10a](#). We
 1278 see that the distributions are similar for energies before 8 MeV but there is an excess of event recon-
 1279 structed with energies around 9 MeV while a lack of them for 10 MeV. The neural network seems to
 1280 learn the energy distribution and learn that it exist almost no event with an energy inferior to 1.022
 1281 MeV and not event with an energy superior to 10 MeV.

1282 The first observation is a physics phenomena: for a positron, its minimum deposited energy is the
 1283 mass energy coming from its annihilation with an electron 1.022 MeV. There is a few event with
 1284 energies inferior to 1.022 MeV, in those case the annihilation gammas or even the positron escape the
 1285 detector. The deposited energy in the LS is thus only a fraction of the energy of the event.

1286 The second observation is indeed true in this dataset but has no physical meaning, it is an arbitrary
 1287 limit because the physics region of interest is mainly between 1 and 9 MeV of deposited energy
 1288 (figure [2.2](#)). By learning the energy distribution, the CNN pull event from the border of it to more
 1289 central value. That’s why the energy resolution is better: the events are pulled in a small energy
 1290 region , thus a small variance but the bias become very high (figure [4.8a](#)).

1291 This behavior also explain the heavy bias at low energy in figure [4.8a](#). The energy bias of the CNN if
 1292 fairly constant over the energy range, it is interesting to note that the energy bias depending on the
 1293 radius is a bit worse than the classical method.

1294 **Vertex reconstruction**

1295 For the vertex reconstruction we do not study x , y and z independently but we use R as a proxy
 1296 observable. Figure [4.9](#) shows the error distribution of the different vertex coordinates. We see that
 1297 R errors and biases are slightly superior to the cartesian coordinates, thus R is a conservative proxy
 1298 observable to discuss the subject of vertex reconstruction.

1299 The comparison of radius reconstruction between the classical algorithm and “gen_30” are presented
 1300 in the figures [4.8c](#), [4.8d](#), [4.8e](#) and [4.8f](#).

1301 Radius reconstruction is worse than the classical algorithms in all configuration. In energy, figure
 1302 [4.8c](#), where we see a degradation of almost 20cm over the energy range.

1303 When looking over the true event radius, figure [4.8d](#), we lose between 30 and 45cm of resolution.
 1304 The performances are the best for central and radial event.

1305 The precision also worsen when looking at the edge of the image $\theta \approx 0$, $\theta \approx 2\pi$ respectively the
 1306 top and bottom of the image, and when $\phi \approx -\pi$ and $\phi \approx \pi$ respectively the left and right side of
 1307 the image. This is the confirmation that the deformation of the image is problematic for the event
 1308 reconstruction.

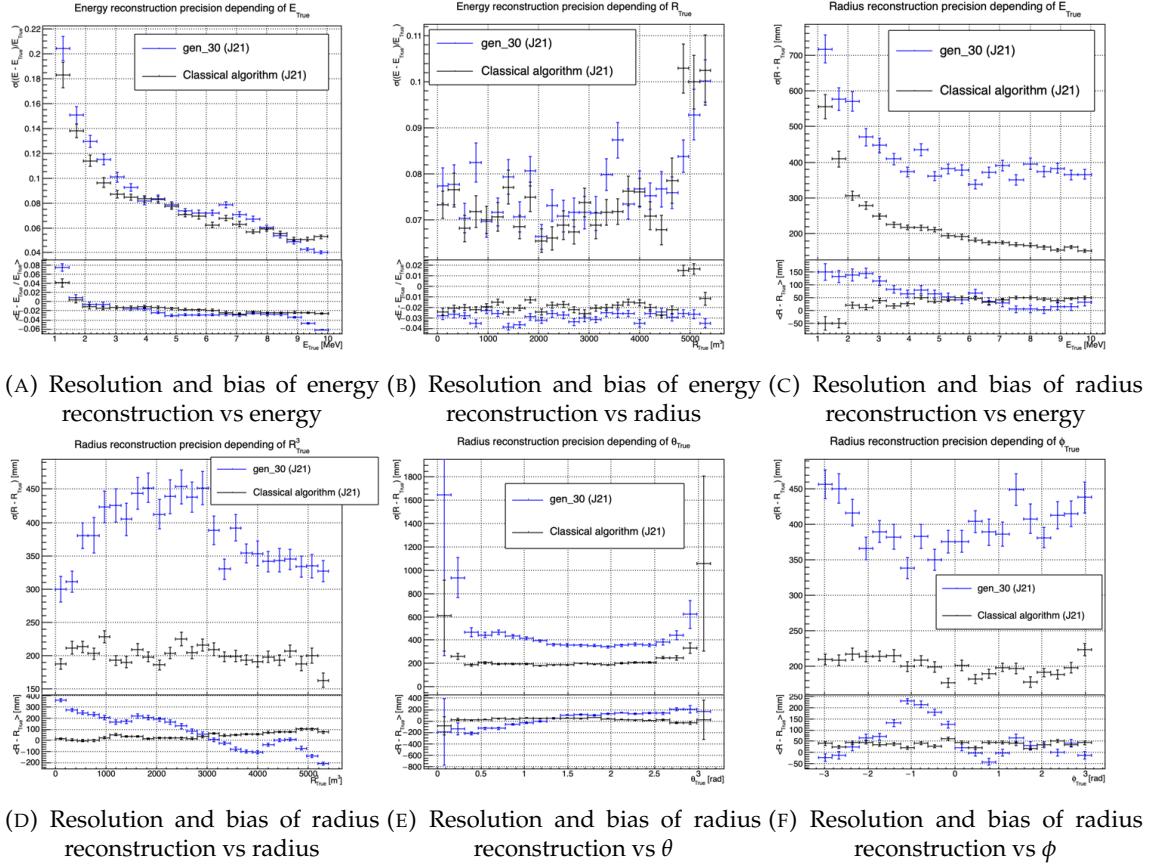


FIGURE 4.8 – Reconstruction performance of the “gen_30” model on J21 data and its comparison to the performances of the classic algorithm “Classical algorithm” from [66]. The top part of each plot is the resolution and the bottom part is the bias.

1309 The bias in radius reconstruction is about the same order of magnitude depending of the energy but
1310 is of opposite sign. As for the energy, this behavior is studied in more details in section 4.4.2. Over
1311 radius, θ and ϕ the bias is inconsistent, sometimes event better than the classical reconstruction but
1312 can also be much worse than the classical method. This could come from the specialisation of some
1313 filters in the convolutional layers for specific part of the detector that would still work “correctly” for
1314 other parts but with much less precision.

1315 4.4.2 J21 Combination of classic and ML estimator

As it has been presented in previous section, there is instances where the reconstructed energy and vertex behaves differently between the neural network and the classic algorithm. For instance, if we look at figure 4.8c, we see that while the CNN tend to overestimate the radius at low energy while the classical algorithm seems to underestimate it. Let’s designate the two reconstruction algorithms as estimator of X , the truth about the event in the phase space (E, x, y, z) . The CNN and the classical algorithm are respectively designated as $\theta_N(X)$ and $\theta_C(X)$.

$$E[\theta_N] = \mu_N + X; \text{Var}[\theta_N] = \sigma_N^2 \quad (4.7)$$

$$E[\theta_C] = \mu_C + X; \text{Var}[\theta_C] = \sigma_C^2 \quad (4.8)$$

1316 where μ is the bias of the estimator and σ^2 its variance.

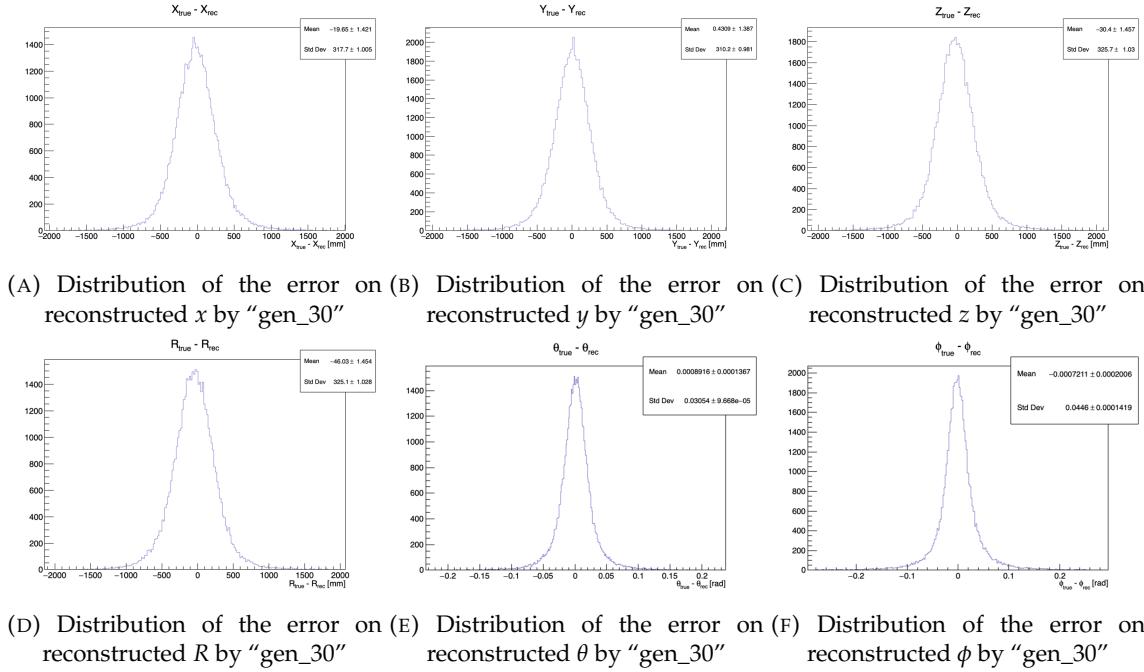


FIGURE 4.9 – Error distribution of the different component of the vertex by "gen_30". The reconstructed component are x , y and z but we see similar behavior in the error of R , θ and ϕ .

1317 Now if we were to combine the two estimators using a simple mean

$$\hat{\theta}(X) = \frac{1}{2}(\theta_N(X) + \theta_C(X)) \quad (4.9)$$

then the variance and mean would follow

$$E[\hat{\theta}] = \frac{1}{2}E[\theta_N] + \frac{1}{2}E[\theta_C] \quad (4.10)$$

$$= \frac{1}{2}(\mu_N + X + \mu_C + X) \quad (4.11)$$

$$= \frac{1}{2}(\mu_N + \mu_C) + X \quad (4.12)$$

$$\text{Var}[\hat{\theta}] = \frac{1}{4}\sigma_N^2 + \frac{1}{4}\sigma_C^2 + 2 \cdot \frac{1}{4} \cdot \sigma_{NC} \quad (4.13)$$

$$= \frac{1}{4}\sigma_N^2 + \frac{1}{4}\sigma_C^2 + \frac{1}{2} \cdot \sigma_{NC} \quad (4.14)$$

$$= \frac{1}{4}\sigma_N^2 + \frac{1}{4}\sigma_C^2 + \frac{1}{2} \cdot \sigma_N \sigma_C \rho_{NC} \quad (4.15)$$

1318 Where σ_{NC} is the covariance between θ_N and θ_C and ρ_{NC} their correlation.

1319 We see immediately that if the two estimators are of opposite bias, the bias of the resulting estimator
1320 is reduced. For the variance, it depends of ρ_{NC} but in this case if σ_C^2 is close to σ_N^2 then even for
1321 $\rho_{NC} \lesssim 1$ then we can gain in resolution.

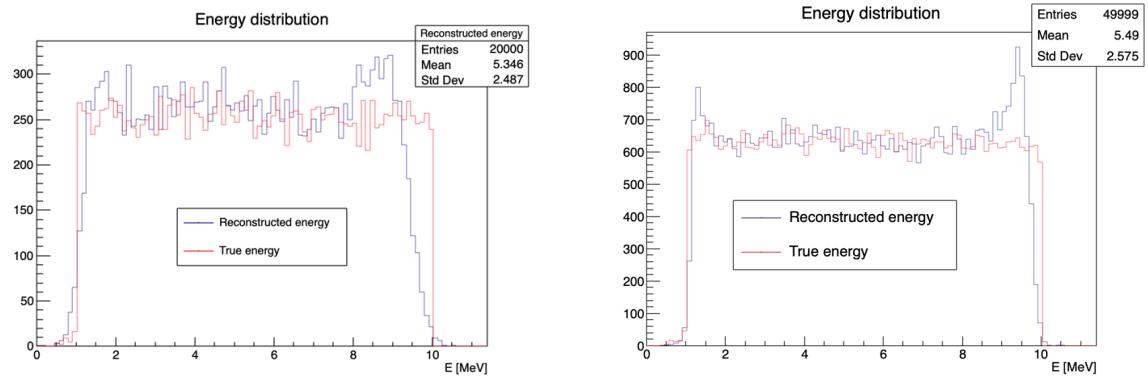
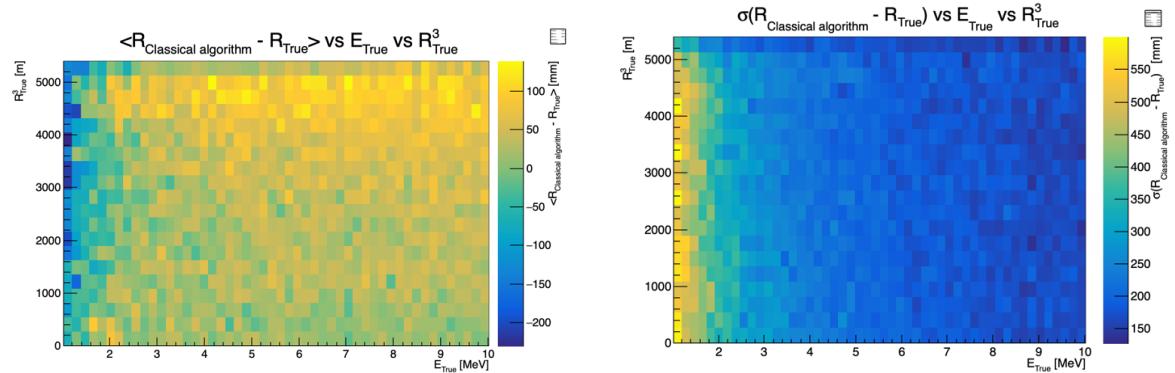


FIGURE 4.10

FIGURE 4.11 – Radius bias (on the left) and resolution (on the right) of the classical algorithm in a E, R^3 grid

1322 By generalising the equation 4.9 to

$$\hat{\theta}(X) = \alpha\theta_N + (1 - \alpha)\theta_C; \alpha \in [0, 1] \quad (4.16)$$

1323 we can determine an optimal α for two combined estimators. The estimators with the smallest
1324 variance

$$\alpha = \frac{\sigma_C^2 - \sigma_N\sigma_C\rho_{NC}}{\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC}} \quad (4.17)$$

1325 and the estimator without bias

$$\alpha = \frac{\mu_C}{\mu_C - \mu_N} \quad (4.18)$$

1326 See annex A for demonstration.

1327 Its pretty clear from the results shown in figure 4.8 that the bias, variances and correlation are not
1328 constant across the (E, R^3) phase space. We thus compute those parameters in a grid in E and R^3 for
1329 the following results as illustrated in 4.11.

1330 The map we are using are composed of 20 bins for R^3 going from 0 to 5400 m^3 (17.54 m) and 50 bins
1331 in energy ranging from 1.022 to 10.022 MeV . In the case where we are outside the grid, we use the
1332 closest cell.

The performance of this weighted mean is presented in figure 4.12. We can see that even when the CNN resolution is much worse than the classical algorithm, it can still bring some information thus improving the resolution. This comes from the correlation of the reconstruction error to be smaller than 1 as presented in figure 4.13. We even see some anticorrelation in the radius reconstruction for High radius, high energy, event.

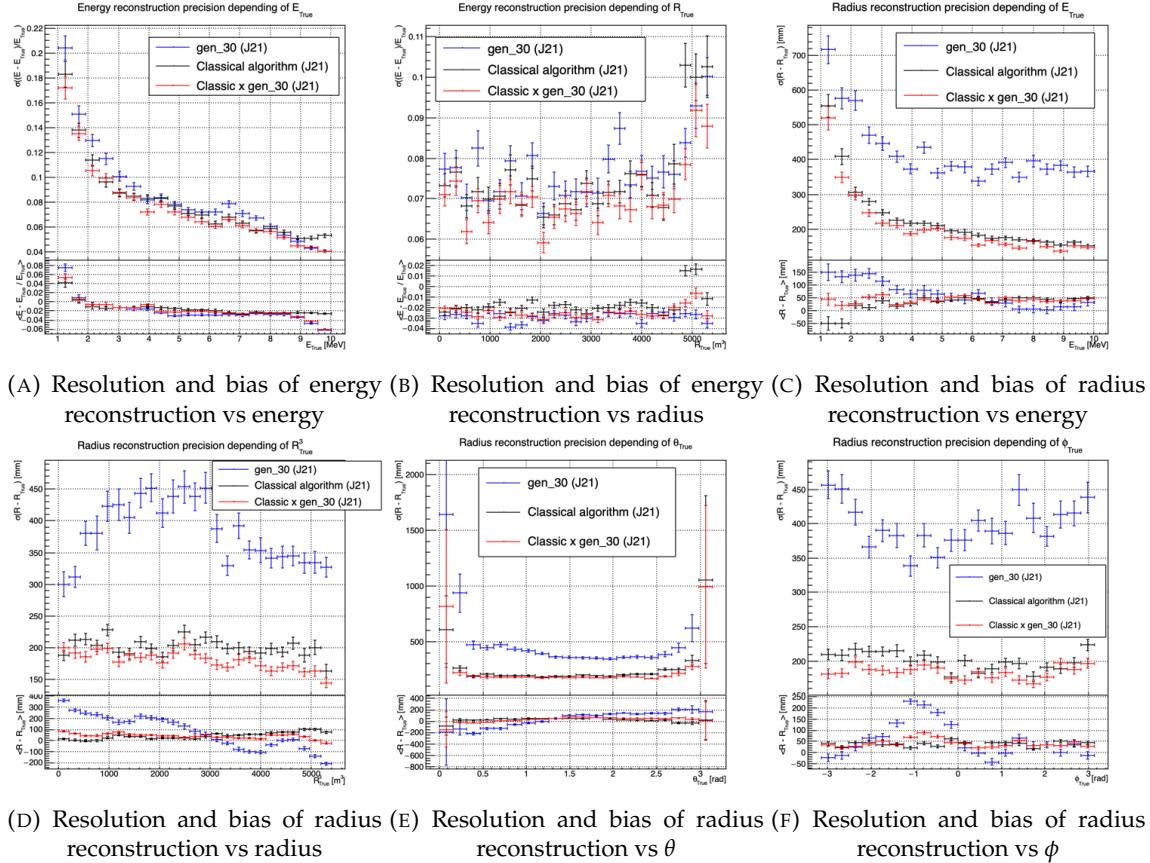


FIGURE 4.12 – Reconstruction performance of the “gen_30” model on J21, the classic algorithm “Classical algorithm” from [66] and the combination of both using weighted mean. The top part of each plot is the resolution and the bottom part is the bias.

This technique is not suited for realistic reconstruction, we rely too much on the knowledge of the resolution, bias and correlation between the two methods. While this is possible to determine using simulated data or calibration sources, the real data might differ from our model and we would need to really well understand the behavior of the two system. But this is an excellent tool to indicate potential improvements to algorithms and reconstruction methods, showing with this results a potential upper limit to the reconstruction performances.

4.4.3 J23 results

The J21 simulation is fairly old and newer version, such as J23, include refined measurements of the light yield, reflection indices of materials of the detector, structural elements such as the connecting structure and more realistic dark noise. Additionally, the trigger, waveform integration and time window are defined using the algorithms that will ultimately be used by the collaboration to process real physics events.

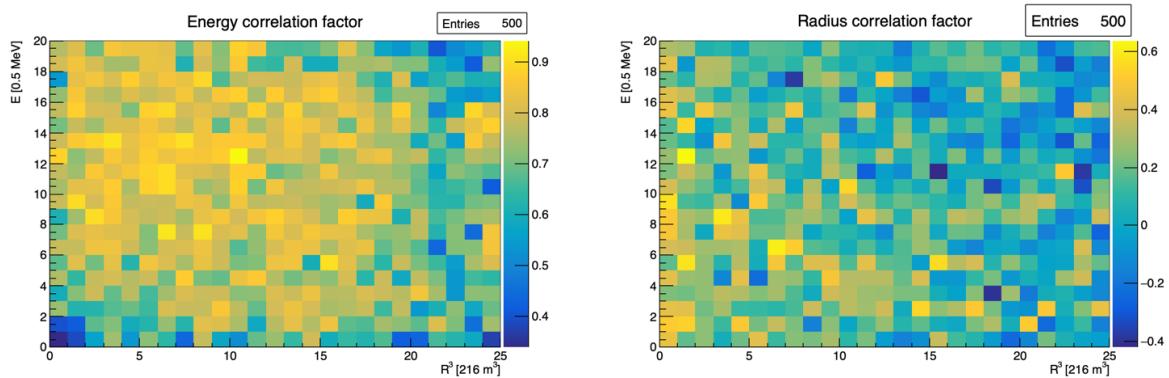


FIGURE 4.13 – Correlation between CNN and classical method reconstruction (on the left) for energy and (on the right) for radius in a E, R^3 grid

We retrained the models defined in 4.2.1 on the J23 data and used the same selection procedure. The results from the best architecture, “gen_42”, are presented in figure 4.14. Following the table 4.1, “gen_42” is defined as:

— “gen_42”: $N_{blocks} = 3$, $N_{channels} = 64$, FCDNN configuration: $4096 * 2$, Loss :– $E + V$

1354 Energy reconstruction

The results of the energy reconstruction are presented in figures 4.14a and 4.14b. Similarly to what we seen for J21, the resolution is close to the one of the classical algorithm with the exception of the start and end of the spectrum. This come from “gen_42” learning the shape of the distribution and pulling events from the extreme energies, like 1 and 10 MeV, to more common seen energy, like 2 and 9 MeV as illustrated in figure 4.10b. The bias disappear with the exception of low and high energy events.

1361 Vertex reconstruction

The vertex reconstruction, presented in figures 4.14c, 4.14d, 4.14e and 4.14f is not yet to the level of the classical reconstruction but the degradation is smaller than for “gen_32” being at most a difference of 15cm of resolution and closing to the performance of the classical algorithm in the most favourable condition. “gen_42” has also very little bias in comparison with the classical method with the exception of the transition to the TR area and at the very edge of the detector.

Unfortunately could not rerun the classical algorithms over the J23 data, as the algorithm was optimised for J21 and was not included and maintained over J23. The combination method need for the two estimators to be run on the same set of event, which was impossible without the classical algorithm being maintained for J23.

Overall the resolution improved over the transition from J21 to J23, effect probably coming from a more complete and rigorous simulation.

1373 4.5 Conclusion and prospect

The CNN is a fine tool for event reconstruction in JUNO, and while the reconstruction performances are satisfactory, it show its limitation, the main one concerning the data representation. A lot of

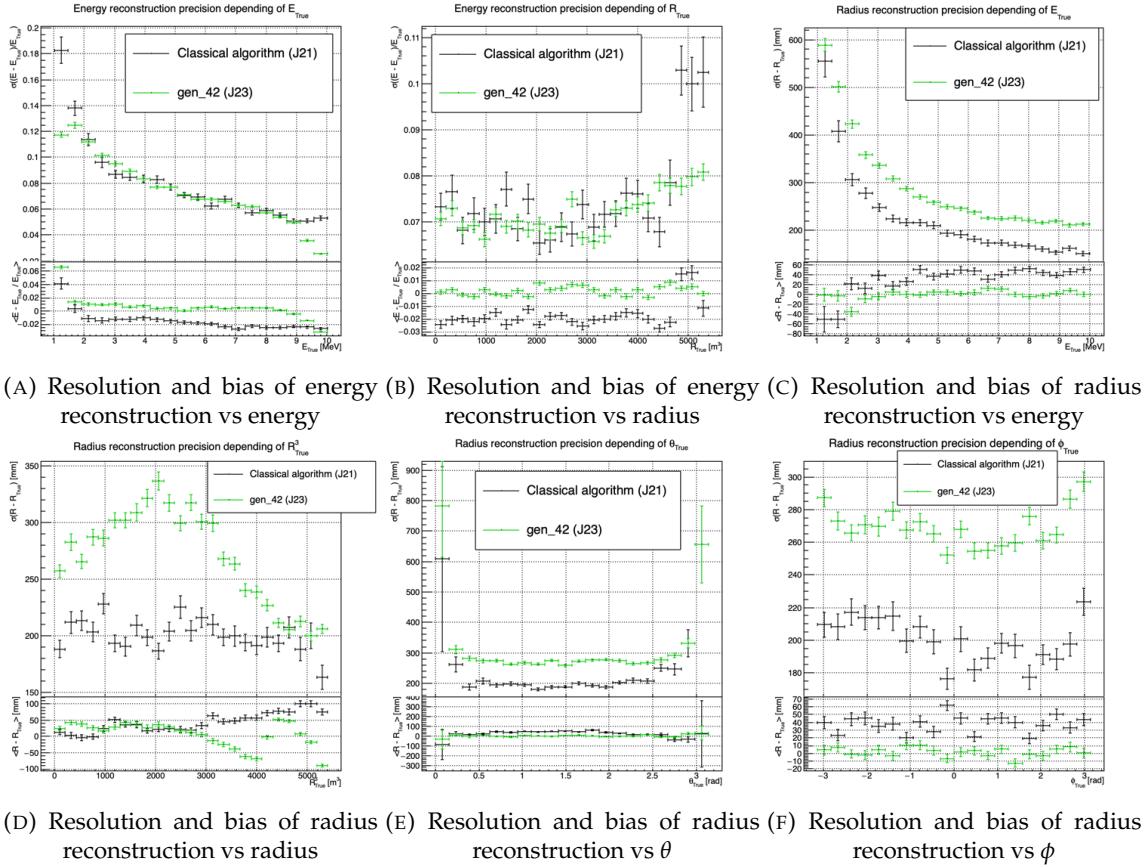


FIGURE 4.14 – Reconstruction performance of the “gen_42” model on J23 data and its comparison to the performances of the classic algorithm “Classical algorithm” from [66]. The top part of each plot is the resolution and the bottom part is the bias.

1376 training time and resources is consumed going and optimizing over pixel with no physical meaning,
 1377 the NN needs to optimized itself to take into account edges cases such as event at the edge of the
 1378 image and deformation of the charge distribution.

1379 Those problems could be circumvented, we could imagine a two part CNN where the first part
 1380 reconstruct the θ and ϕ spherical coordinates and then rotate the image to locate the event in the
 1381 center of the image. The second part, from this rotated image, would reconstruct the radius and
 1382 energy of the event.

1383 To overcome the problematic of the aggregation of PMT time information and the meaning of the
 1384 time channel in case of no hit, we could transform this channel into a dimension. This would results
 1385 in an image with multiple charge channels, each one representing the charge sum in a time interval.

1386 In this thesis, we decided to solve those problem by moving away from the 2D image representation,
 1387 looking into the graph representation and the Graph Neural Network (GNN). This is be the subject
 1388 of the next chapter.

¹³⁸⁹ **Chapter 5**

¹³⁹⁰ **Graph representation of JUNO for
IBD reconstruction**

¹³⁹²

*"The Answer to the Great Question of Life, the Universe and
Everything is Forty-two"*

Douglas Adams, The Hitchhiker's Guide to the Galaxy

¹³⁹³ We previously showed, in chapter 4, that neural networks are relevant as reconstruction tools in
¹³⁹⁴ JUNO. Even if they show worse performances, the combination with classical estimators could still
¹³⁹⁵ bring improvements. We discussed the use of Convolutional Neural Network (CNN) in the previous
¹³⁹⁶ chapter and their limitations, more specifically the limitation of the image as data representation for
¹³⁹⁷ the experiment.

¹³⁹⁸ In this chapter we propose to use a Graph Neural Network (GNN), a Neural Network specialized to
¹³⁹⁹ process graph as presented in section 3.2.3, to overcome those limitations.

¹⁴⁰⁰ **5.1 Motivation**

¹⁴⁰¹ As explained in chapter 2 the JUNO sensors, the Large Photomultipliers (LPMT) and Small Pho-
¹⁴⁰² tomtmultipliers (SPMT), are arranged on a spherical plane. When trying to represent this plane as a
¹⁴⁰³ 2D image, due to the inherent problem of the projection, some part of the image are distorted and
¹⁴⁰⁴ part of the image do not have any physical meaning (see section 4.2.2). A way to represent the data
¹⁴⁰⁵ without inducing deformation is the graph, an object composed of a collection of nodes and edges
¹⁴⁰⁶ representing the relation between the nodes.

¹⁴⁰⁷ From this graph representation, we can construct a neural network that will process the data while
¹⁴⁰⁸ keeping some interesting properties. For example the rotational invariance, i.e. the energy and
¹⁴⁰⁹ radius of the event do change by rotation our referential. For more details see section 3.2.3. Graph
¹⁴¹⁰ representation also has the advantage to be able to encode global and higher order informations.

¹⁴¹¹ An approach was already proposed in JUNO by Qian et al. [42] where each nodes of the graph are
¹⁴¹² like pixels, they represent geometric region of the detector and are connected with their neighbours.
¹⁴¹³ The LPMT informations are then aggregated on those nodes. The network then process the data
¹⁴¹⁴ using the equivalent of convolution but on graph [49].

¹⁴¹⁵ In this work we want to take a step further in the graph representation by including the SPMT and
¹⁴¹⁶ including a maximum of raw informations.

5.2 Data representation

In an ideal world we would like to have every PMTs represented as node in the graph, each PMT being hit is an informations but the fact that PMTs were not hit is also an important information. It's by being aware of the whole of the system that we are able to give meaning to a subpart. As a reminder, in the Central Detector (CD), JUNO will posses 17612 LPMTs and 25600 SPMTs for a total of 43212 PMTs. This amount of information in itself is still manageable by modern computer if it were to be used in a neural network but when defining the relations between the nodes, it become a bit more tricky.

Excluding self relation and considering the relation to be undirected, the edge from A to B is the same from B to A , the amount of necessary edges is given by $\frac{n(n-1)}{2}$ which for 43212 PMTs amount for 933'616'866 edges. If we encode an information with double precision (64 bits) in what we call an adjacency matrix, each information we want to encode in the relation would consume 4 GB of data. When adding the overhead due to gradient computation during training, this would put us over the memory capacity of a single V100 gpu card (20 GB of memory). We could use parallel training to distribute the training over multiple GPU but we considered that the technical challenge to deploy this solution was not worth the trouble.

The option of connecting PMTs node only to their neighbours could be tempting to reduce the number of edge, but this solution does not translate well in term of internal representation in memory. Edges of sparsely connected nodes can be stored in efficient manner in a sparse matrix but the calculation in itself would often results in the concretization of the full matrix in memory, resulting in no memory gain during training.

We finally decided of a middle ground where we define three *families* of nodes:

- The core of the graph is composed of nodes representing geometric regions of the detector. We call those nodes **mesh** nodes. Those mesh nodes are densely connected to each other. We keep their number low to gain in memory consumption.
- All the fired PMTs, that have been hit, will be represented as nodes. We call those node **fire**. Fired nodes are connected to the mesh they geometrically belong.
- A final node which will hold global information about the detector and on which we will read the interaction vertex and energy. It's designated as the **I/O** node for input/output. This node will be connected to every mesh nodes.

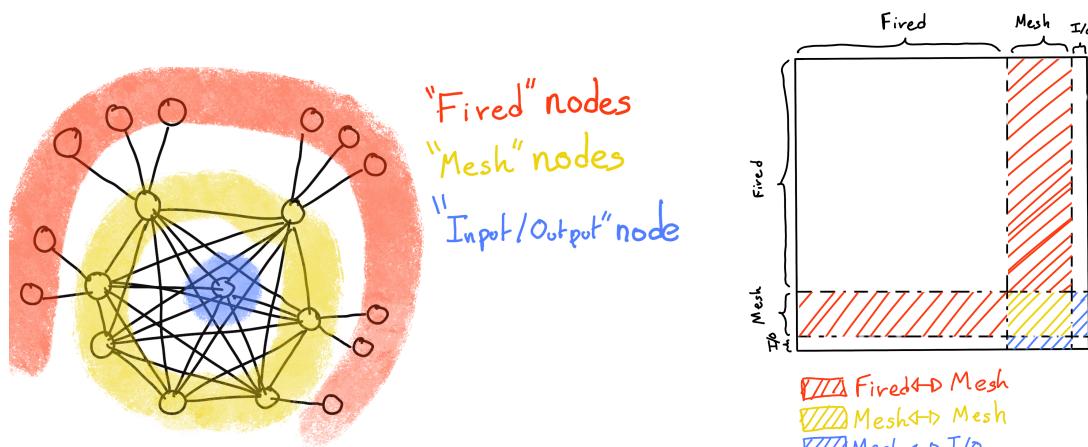
Those nodes and their relations are illustrated in figure 5.1a. From this representation, we end up with three distinct adjacency adjacency matrix

- A $N_{\text{fire}} \times N_{\text{mesh}}$ adjacency matrix, representing the relations between fired and mesh. Those relations are undirected.
- A $N_{\text{mesh}} \times N_{\text{mesh}}$ adjacency matrix, representing the relation between meshes. Those relation are directed.
- A $N_{\text{mesh}} \times 1$ adjacency between the mesh and I/O nodes. Those relations are undirected.

The adjacency matrix representing those relation is illustrated in figure 5.1b.

The mesh segmentation is following the Healpix segmentation [76]. This segmentation offer the advantage that almost each mesh have the same number of direct neighbours and it guarantee that each mesh represent the same extent of the detector surface. The segmentation can be infinitely subdivided to provide smaller and smaller pixels. The number of pixel follow the order n with $N_{\text{pix}} = 12 \cdot 4^n$. This segmentation is illustrated in figure 5.2. To keep the number of mesh small, we use the segmentation of order 2, $N_{\text{pix}} = 12 \cdot 4^2 = 192$.

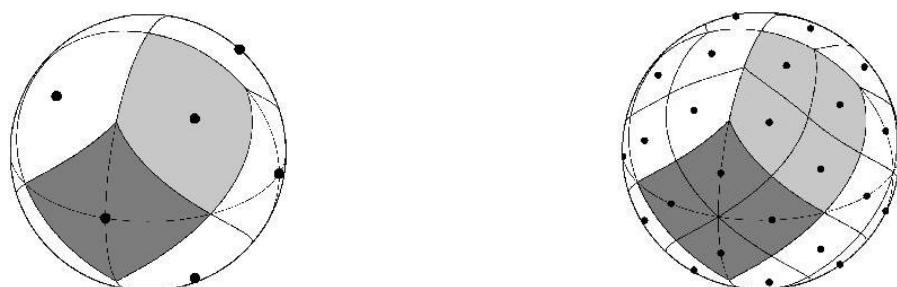
We decided on having the different kind of nodes **mesh (M)**, **fire (F)** and **I/O** have different set of features. The features used in the graph are presented in figure 5.3. Most of the features are low level informations such as the charge or time information but we include some high order features such as



(A) Illustration of the different nodes in our graphs and their relations.

(B) Illustration of what a dense adjacency matrix would look like and the part we are really interested in. Because Fired → Mesh and Mesh → I/O relations are undirected, we only consider in practice the top right part of the matrix for those relations.

FIGURE 5.1

FIGURE 5.2 – Illustration of the healpix segmentation. **On the left:** A segmentation of order 0. **On the right:** A segmentation of order 1

- 1465 1. P_l^h : Is the normalized power of the l th spherical harmonic. For more details about spherical
1466 harmonics in JUNO, see annex B.

2. \mathbb{A} and \mathbb{B} are informations that represent the likeliness of the interaction vertex to be on the segment between the center of two meshes.

$$\mathbb{A}_{ij} = (\vec{j} - \vec{i}) \cdot \frac{\vec{l}_1}{D_{ij}} + \vec{i} \quad (5.1)$$

$$\mathbb{B}_{ij} = \frac{Q_i}{Q_2} \left(\frac{\vec{l}_2}{\vec{l}_1} \right)^2 \quad (5.2)$$

$$l_1 = \frac{1}{2}(D_{ij} - \Delta t \frac{c}{n}) \quad (5.3)$$

$$l_2 = \frac{1}{2}(D_{ij} + \Delta t \frac{c}{n}) \quad (5.4)$$

1467 where \vec{i} is the position vector of the mesh i , D_{ij} is the distance between the center of the meshes
1468 i and j , Q_i the sum of charges on the mesh i , $\Delta t = t_i - t_j$ where t_i the earliest time on the mesh
1469 i and n the optical index of the LS. \mathbb{A} is the vertex between center of meshes distance ratio
1470 between i and j based on the time information. For \mathbb{B} , the charge ratio evolve with the square
1471 of the distance, so the mesh couple with the smallest \mathbb{B} should be the one with the interaction
1472 vertex between its two center.

Nodes			Edges		
Fixed	Mesh	I/O	Fixed \rightarrow Mesh	Mesh \rightarrow Mesh (1) \rightarrow Mesh (2)	Mesh \rightarrow I/O
Q	$\langle Q_m \rangle$	$\langle x \rangle$	$X - X_m$	$X_{m1} - X_{m2}$	$\langle x \rangle - x_m$
t	$6Q_m$	$\langle y \rangle$	$Y - Y_m$	$Y_{m1} - Y_{m2}$	$\langle y \rangle - y_m$
X	$\min(t_m)$	$\langle z \rangle$	$Z - Z_m$	$Z_{m1} - Z_{m2}$	$\langle z \rangle - z_m$
Y	$\max(t_m)$	ΣQ	$t - \min(t)$	$\min(t_1) - \min(t_2)$	$\Sigma Q_m / \Sigma Q$
Z	$6t_m$	$P_l^h; l \in [0, 8]$	$Q / \Sigma Q_m$	$\langle Q_{m1} \rangle - \langle Q_{m2} \rangle$ $\langle Q_{m1} \rangle + \langle Q_{m2} \rangle$	$\langle t_m \rangle$
LPMT: 1 SPMT: -1	X_m Y_m Z_m			$D_{m1 \rightarrow m2}^{-1}$ \mathbb{A} \mathbb{B}	

Q is the charge [nPE]
 t is the time [ns]
 X, Y, Z are the coordinates [m]
 Q_m, t_m are the set of charge and time in a mesh
 X_m, Y_m, Z_m the coordinates of the center of the mesh
 $\langle x \rangle, \langle y \rangle, \langle z \rangle$ the position of the charge barycenter.

FIGURE 5.3 – Features held by the nodes and edges in the graph. $D_{m1 \rightarrow m2}^{-1}$ is the inverse of the distance between two mesh center. The features P_l^h , \mathbb{A} and \mathbb{B} are detailed in section 5.2

1473 Because our different nodes do not have the same number of features, they live in different spaces.
1474 Most library and public algorithms available are designed with node living in the same space in
1475 mind, we thus had to develop a custom message passing algorithm.

5.3 Message passing algorithm

1477 As introduced in previous section and in figure 5.3, our graphs nodes and edges will have different
1478 number of features depending on their nature, meaning that we cannot have a single message passing
1479 function. We thus need to define a message passing function for each transition inside or outside

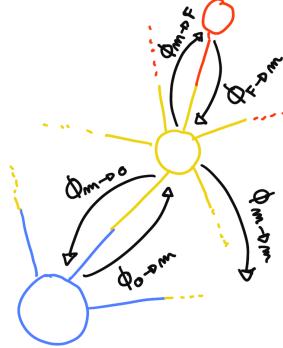


FIGURE 5.4 – Illustration of the different update function needed by our GNN

¹⁴⁸⁰ a family. Using the notation presented in section 3.2.3

$$n_i^{k+1} = \phi_u(n_i^k, \square_j \phi_m(n_i^k, n_j^k, e_{ij}^k)); n_j \in \mathcal{N}_i' \quad (5.5)$$

we need to define

$$\phi_{u;f \rightarrow m} \phi_{m;f \rightarrow m} \quad (5.6)$$

$$\phi_{u;m \rightarrow f} \phi_{m;m \rightarrow f} \quad (5.7)$$

$$\phi_{u;m \rightarrow m} \phi_{m;m \rightarrow m} \quad (5.8)$$

$$\phi_{u;m \rightarrow io} \phi_{m;m \rightarrow io} \quad (5.9)$$

$$\phi_{u;io \rightarrow m} \phi_{m;io \rightarrow m} \quad (5.10)$$

¹⁴⁸¹ to update the nodes after each layers as illustrated in figure 5.4. We would also need update function
¹⁴⁸² for the edges but for the sake of technical simplicity in this work, we will limit ourself to the nodes
¹⁴⁸³ update. A wide variety of message passing algorithm exists, with different use cases and goal behind
¹⁴⁸⁴ them. To stay generalist and to match to the best the specificity of our architecture, we implement
¹⁴⁸⁵ the following algorithm:

$$\phi_u := I_{i'}^{n'} = I_i^n A_{i',e}^i W_n^{e,n'} + I_i^n S_n^{n'} + B^{n'} \quad (5.11)$$

¹⁴⁸⁶ using the Einstein summation notation. I_i^n is the tensor holding the nodes informations with i
¹⁴⁸⁷ the node index and n the feature index. n represent the features of the previous layer and n' the
¹⁴⁸⁸ features of this layer. $A_{i',e}^i$ is the adjacency tensor, discussed in the previous section, representing the
¹⁴⁸⁹ connection between the node i' and the node i , each connections holding the features indexed by e .
¹⁴⁹⁰ The learnable weights are composed of:

- ¹⁴⁹¹ — The tensor $W_n^{e,n'}$ which represent the passage from the previous feature domain n , the previous
¹⁴⁹² layer, to the current domain n' , this layer knowing the relation e .
- ¹⁴⁹³ — $B^{n'}$ which is a learnable bias tensor on the new features n' .
- ¹⁴⁹⁴ — $S_n^{n'}$ which can be viewed as a self loop relation where the node update itself based on the
¹⁴⁹⁵ previous layer informations.

¹⁴⁹⁶ If a node have neighbours in different families, the different $I_{i'}^{n'}$ coming from the different ϕ_u are
¹⁴⁹⁷ summed.

$$I_{i'}^{n'} = \sum_{\mathcal{N}} \phi_{u,\mathcal{N}} \quad (5.12)$$

¹⁴⁹⁸ where \mathcal{N} are the neighbouring family and $\phi_{u,\mathcal{N}}$ the update function between the target node family
¹⁴⁹⁹ and the neighbour \mathcal{N} family.

¹⁵⁰⁰ We thus have a S , W and B for each of the ϕ_u function we defined above. The IAW sum can be seen

as the ϕ_m function and $IS + B$ as the second part of the phi_u function. Interestingly, the number on learnable weight in those layer is independent of the number of nodes in each family and depends solely on the number of features on the nodes and the edges.

The expression above only update the node features. We could update the edges, using the results of ϕ_m for example, but for technical simplicity we only update the nodes and keep the edges constant.

This operation of message passing is the constituent of our message passing layer, designed in this work as *JWGLayer*. To this layer, we can adjoin an activation function such as *PReLU*

$$I_i^{n'} = PReLU \left(\sum_{\mathcal{N}} I_i^n A_{i',e}^i W_n^{e,n'} + I_i^n S_n^{n'} + B^{n'} \right) \quad (5.13)$$

5.4 Data

For this study we will be using a 1M positrons event dataset, uniformly distributed in energy with $E_k \in [0, 9]$ MeV and uniformly distributed in the detector. Those events come from the JUNO official simulation version J23.0.1-rc8.dc1 (released the 7th January 2024). All the event are *calib* level, with simulation of the physics, electronics, digitizations and triggers. 900k events will be used for the training, 50k for validation and loss monitoring and 50k for the results analysis in section 5.8. Each events is between 2k and 12k fired PMTS, resulting in fired nodes being the largest family in our graphs in all circumstances as illustrated in figure 5.5c.

As expected, by comparing the scale between the figure 5.5a and 5.5b we see that the LPMT system is predominant in term of informations in our data. The number of PMT hits grow with energy but do not reach 0 for low energy event due to the dark noise contribution which seems to be around 1000 hits per event for the LPMT system (left limit of figure 5.5a) and around 15 hits per event for the SPMT system (left limit of figure 5.5b) which is consistent with the results show in section 4.2.2.

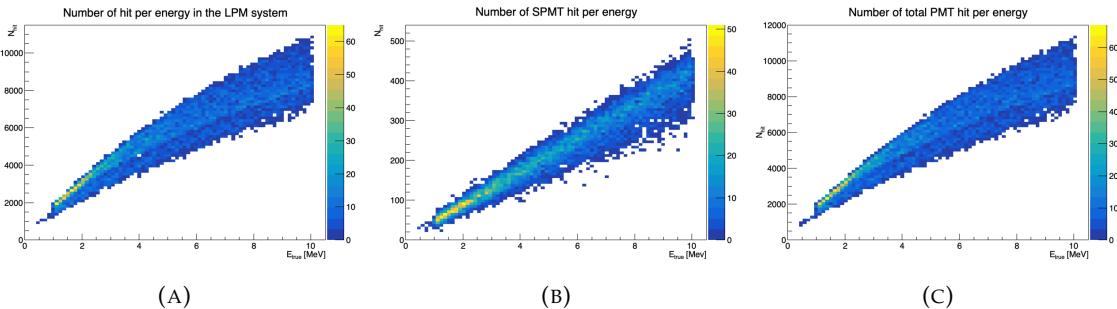


FIGURE 5.5 – Distribution of the number of hits depending on the energy. **On the right:** for the LPMT system. **In the middle :** for the SPMT system. **On the left:** For both system.

The structure seen in the distribution in figure 5.5a comes from the shape of the number of hits depending on the radius as shown in figures 5.6a and 5.6b where the number of hit decrease with radius. It is important to understand that this is not representative of the number of PE per event and the decrease in hits over the radius means that the PE are just more concentrated in a smaller number of PMTs.

No quality cut is applied here, we rely only on the trigger system. It means that event that would not trigger are not present in the dataset but for events that triggered twice, it happens rarely, the two trigger are considered as two separate event.

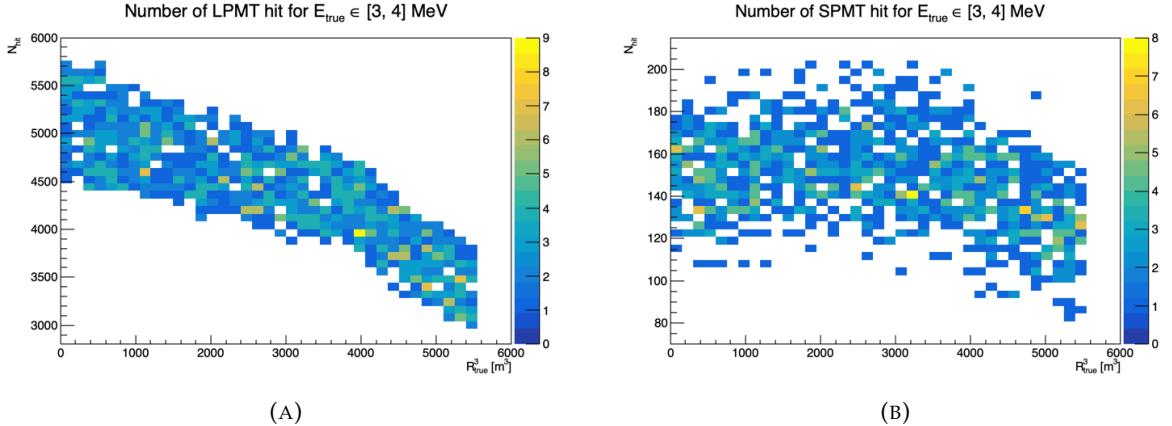


FIGURE 5.6 – Distribution of the number of hits depending on the radius. **On the right:** for the LPMT system. **On the right :** for the SPMT system. To prevent the superposition of structure of different scales we limit ourselves to the energy range $E_{true} \in [0, 9]$.

5.5 Model

In this section we'll discuss the different layer composing the final version of the model. As introduced above, each JWGLayer is defined by the number of features on the nodes and edges of the output graph, assuming it takes as input the graph from the precedent layer. For simplicity, when discussing a graph configuration, it will be presented as follow: { N_f , N_m , N_{IO} , $N_{f \rightarrow m}$, $N_{m \rightarrow m}$, $N_{m \rightarrow f}$ } where

- N_f is the number of feature on the fired nodes.
 - N_m is the number of features on the mesh nodes.
 - N_{IO} is the number of features on the I/O node.
 - $N_{f \rightarrow m}$ is the number of features on the edges between the fired and mesh nodes.
 - $N_{m \rightarrow m}$ is the number of features on the edges between two mesh nodes.
 - $N_{m \rightarrow f}$ is the number of features on the edges between the mesh nodes and the I/O node.
- Because we do not change the number of features on the edges, we can simplify the notation to { N_f , N_m , N_{IO} }. As an example, the input graph configuration, following the figure 5.3, is { 6, 8, 13, 5, 8, 5 } or, without the edge features, { 6, 8, 13 }.

The final version of the model, called JWGV8.4.0 is composed of

- An JWGLayer, converting the input graph to { 64, 512, 2048 } with a PReLU activation function.
- 3 resnet layers, each of them composed of
 1. 2 JWG layers with a PReLU activation function. They do not change the dimension of the graph
 2. A sum layer that sums the features in the input graph with the one computed from the JWG layers
- A flatten layer that flatten the features of the I/O and mesh nodes in a vector.
- 2 fully connected layers of 2048 neurons with a PReLU activation function.
- 2 fully connected layers of 512 neurons with a PReLU activation function.
- A final, fully connected layer of 4 neurons acting as the output of the network.

A schematic of the model is presented in figure 5.7.

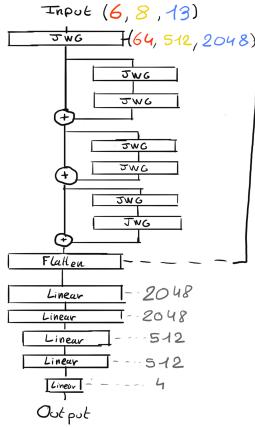


FIGURE 5.7 – Schema of the JWGv8.4.0 architecture, the colored triplet is the graph configuration after each JWG layers

1556 5.6 Training

1557 The optimizer used for training is the Adam optimizer and default hyperparameters ($\beta_1 = 0.9$,
 1558 $\beta_2 = 0.999$ and $\epsilon = 1e-8$) with a learning rate $\lambda = 1e-8$. The training last 200 epochs of 800 steps.
 1559 We use a batch size of 8. The learning rate is constant during the first 20 epochs then exponentially
 1560 decrease with a rate of 0.99. The model saved is the model with the best validation loss during the
 1561 training. The validation is computed over a single batch.

1562 5.7 Optimization

1563 Due to the extensive training time, up to 90h per training on the more complex architectures, and
 1564 the heavy memory consumption of the models that would often exceed the 20GB limit of the V100,
 1565 random search was not a realistic approach to the hyper optimisation. We were able to extend the
 1566 memory limit to 40GB thanks to a local A100 GPU card available at the lab.

1567 The hyperparameters optimization was thus done “by hand”, by looking at the results of the previous
 1568 training and tinker hyperparameters that seems to play a role in the training. During this process,
 1569 the model went into some heavy refactoring. At the start, the message passing algorithm was not
 1570 the one presented above but each ϕ_u and ϕ_m function were FCDNN. The memory consumption and
 1571 gradient vanishing caused is what made us pivot to the final message passing algorithm presented
 1572 above.

1573 Even the features on the graph went under investigation. With the addition of high level observables
 1574 to the mesh and I/O nodes and edge, there was too much possibility to test everything. We went
 1575 with the decision to keep the raw observables in the fired and for the higher order observables
 1576 we tried to take the one that would be difficult for the NN to reconstruct or at least would need
 1577 multiple layer to reproduce. Basically, because the operation in the JWGLayer are linear operation,
 1578 any variables dependent on order > 1 of the input would be candidates. This is why we introduce
 1579 standard deviation, \mathbb{A} , \mathbb{B} and P_l^h for example.

1580 Substantial effort went to the data processing process before the training. Due to the volatile nature
 1581 of the graph features during the optimization, the current code do not take preprocessed data and
 1582 compute the observables, adjacency matrix, etc... on the fly. This data processing is carried out on
 1583 the CPU, using a worker pool to allow for multiprocessing the data. The raw data are coming from

1584 root file produced by the collaboration software, the Event Data Model (EDM) used internally by the
 1585 collaboration [77] had to be interfaced to our code, interface maintained through the evolution of the
 1586 collaboration software. For the harmonic power calculation, we migrated from the Healpix library
 1587 to Ducc0 [78] for a more fine control of the multithreading.

1588 Over the course of the project, the model went over more than 60 different configurations to end on
 1589 the one presented in this chapter.

1590 5.8 Results

1591 The reconstruction performance of “JWGv8.4” are presented in figure 5.9 and compared to the “Omlil-
 1592 rec” algorithm, the official IBD reconstruction algorithm in JUNO. Omlilrec is based on the QTMLR
 1593 reconstruction method that was presented in section 2.6.

1594 We also present the results of the optimal variance combination of the two algorithm labelled as
 1595 “JWG 8.4 x Omlilrec” where the reconstructed target $\hat{\theta}_{\text{target}}$ is the weighted sum of the result of the
 1596 two estimator JWGv8.4 θ_J and Omlilrec θ_O .

$$\hat{\theta} = \alpha\theta_J + (1 - \alpha)\theta_O; \alpha \in [0, 1] \quad (5.14)$$

1597 For more details about the combination and the computation of α , refer to annex A.2.

1598 One thing that need to be addressed before discussing results is that the Omlilrec algorithm do not
 1599 reconstruct the deposited energy E_{dep} but reconstruct the visible energy E_{vis} . The difference between
 1600 those two different observables comes from the event-wise and channel-wise non-linearity, presented
 1601 in 2.3. The multiples energy observables are already discussed in section 4.4. For the following
 1602 results, the systematic bias of Omlilrec that appear due, to the comparison to E_{true} instead of E_{vis} is
 1603 corrected using a 5th degree polynomial

$$\frac{E_{\text{true}}}{E_{\text{rec}}} = \sum_{i=0}^5 P_i E_{\text{true}}^i \quad (5.15)$$

1604 The fitted distribution and the corresponding fit is presented in figure 5.8. The value fitted for this
 1605 correction are presented in table 5.1.

P_0	$1.24541 +/- 0.00585121$
P_1	$-0.168079 +/- 0.00716387$
P_2	$0.0489947 +/- 0.00312875$
P_3	$-0.00747111 +/- 0.000622003$
P_4	$0.000570998 +/- 5.7296e-05$
P_5	$-1.72588e-05 +/- 1.98355e-06$

TABLE 5.1 – Parameters of the 5th degree polynomial used to correct Omlilrec
 reconstructed energy.

1606 Overall, energy and radius resolutions are not on par with Omlilrec. We see from the energy de-
 1607 pendent energy resolution in fig 5.9a that our resolution is a bit more than twice the resolution of
 1608 Omlilrec and the combination brings no improvements. Same observation for the energy resolution
 1609 depending on the radius.

1610 The radius resolution, presented in the figures 5.9c, 5.9d, 5.9e and 5.9f is much worse than the
 1611 Omlilrec one. This comes a bit as a surprise, as the energy reconstruction is dependent on the
 1612 vertex reconstruction to correct for the non-uniformity and non-linearity effect. This mean that
 1613 either the GNN could outperform the classical methods if the vertex was correctly reconstructed,

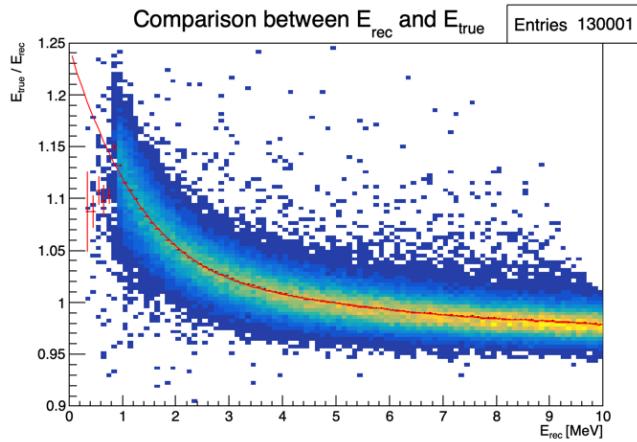


FIGURE 5.8 – Comparison between Omilrec E_{rec} and the true energy E_{true} . The profile of the distribution E_{true} / E_{rec} vs E_{rec} is fitted with a 5th degree polynomial.

1614 or that somewhere the GNN reconstruct the vertex correctly but has trouble to formulate it in x,y,z
 1615 coordinates on the latest layer.

1616 The GNN behaviours are close to Omilrec, indicating that the same information is used in the same
 1617 way by both algorithms, just that the GNN seems to be less fine-tuned than Omilrec. If the precedent
 1618 reasoning is true, it would mean that by adding more parameters, more layer or a higher pixelisation
 1619 of the Healpix representation, the GNN could reach Omilrec performances.

1620 5.9 Conclusion

1621 In this chapter, I present a proposition for a GNN architecture to reconstruct the energy and position
 1622 of the prompt signal of an IBD interaction. The GNN is not competitive in terms of resolution with
 1623 the more classical method Omilrec, which is the state of the art reconstruction method for IBD in the
 1624 JUNO collaboration, but show encouraging results that could be exploited by going further in the
 1625 optimisation of the hyper parameters. The message passing algorithm is still pretty naive and could
 1626 probably be refined for JUNO's need.

1627 Another possible improvement is to find a way to increase the Healpix pixelisation. Through our
 1628 different work on reconstruction and by looking at the different classical methods, it seems that
 1629 the time information is crucial for the vertex reconstruction, and thus for the energy reconstruction.
 1630 While we are keeping every raw informations about the fired PMTs, it is possible that the aggregation
 1631 on mesh nodes could cause the information loss and it has been noticed that allowing more channels
 1632 to the hidden layer mesh nodes improve the resolution. This observation can be compared to the
 1633 convolutional GNN presented section 2.6.3 that has similar performance with the classical method
 1634 with an order 5 Healpix segmentation resulting in 3072 pixels, comforting the need of a finer pixeli-
 1635 sation, or more parameters dedicated to aggregation through an increase of channels on the mesh
 1636 nodes. Both of those improvements require some heavy memory optimisations, distributed training
 1637 or more powerful hardware to address the memory consumption issue.

1638 A final possible improvement would be to go further in the proximity of raw information. The charge
 1639 and time used in the PMTs are extracted from a waveform, we could imagine a world where the full
 1640 PMT waveform in the trigger window would be set of channels on the PMT node.

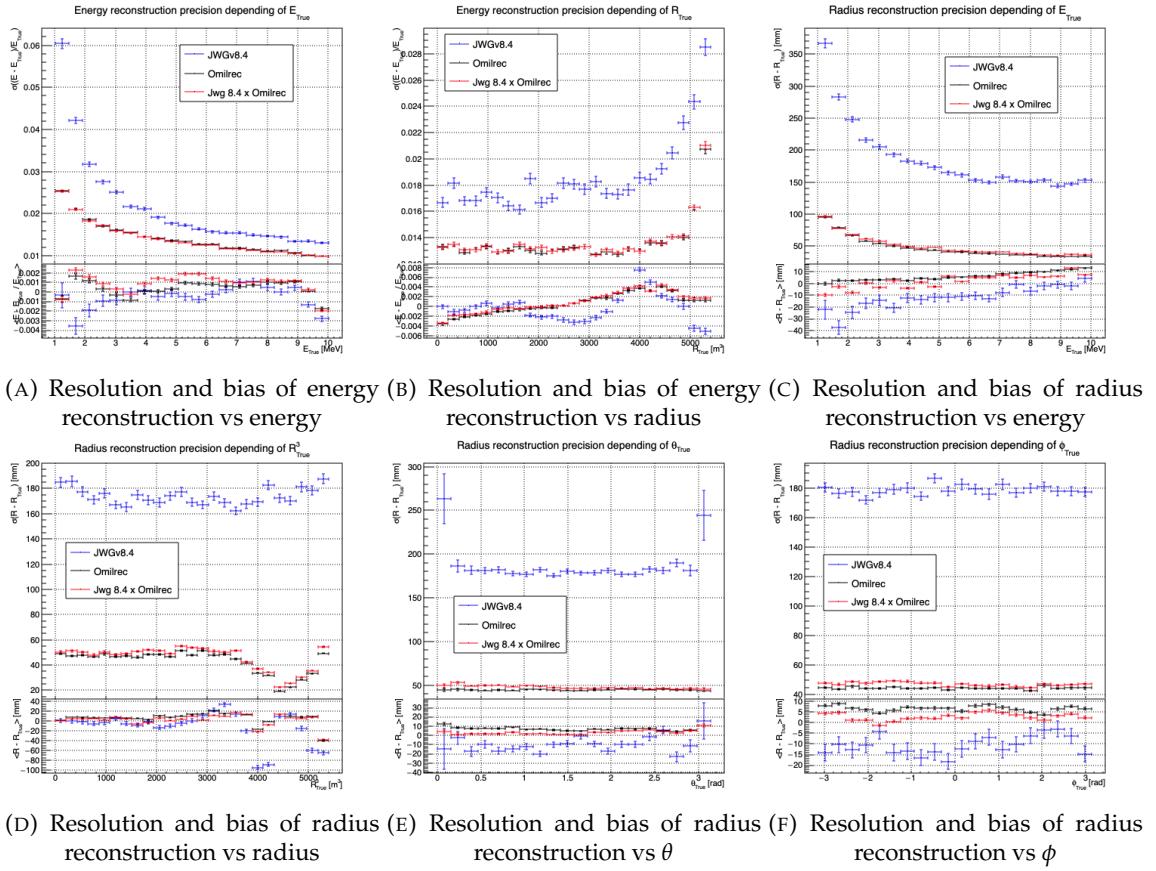


FIGURE 5.9 – Reconstruction performance of the Omilrec algorithm based on QTMLE presented in section 2.6, JWGv8.4 presented in this chapter and the combination between the two as presented in section 4.4.2. The top part of each plot is the resolution and the bottom part is the bias.

¹⁶⁴¹ **Chapter 6**¹⁶⁴² **Reliability of machine learning
methods**
¹⁶⁴³

1644

"Psychohistory was the quintessence of sociology; it was the science of human behavior reduced to mathematical equations. The individual human being is unpredictable, but the reactions of human mobs, Seldon found, could be treated statistically"

Isaac Asimov, Second Foundation

¹⁶⁴⁵ **Chapter 7**

¹⁶⁴⁶ **Joint fit between the SPMT and LPMT
spectra**

¹⁶⁴⁸ “We demand rigidly defined areas of doubt and uncertainty!”

Douglas Adams, *The Hitchhiker’s Guide to the Galaxy*

¹⁶⁴⁹ JUNO is an experiment of precise measurements, where we try to observe small fluctuation in the energy spectrum and have the ambition to achieve sub-percent precision on the oscillation parameters measurement. It is crucial to understand extremely well the reconstruction and the effect we are dealing with. The challenge reside in the standard technology used in the detector, scintillator observed by PMT, but in a scale never seen before, for scintillator volume as for its PMT. Understanding every effect that goes in the detector can become extremely complicated. Being able to compare the results of the same experiment with two systems is thus precious, this is the origin the dual calorimetry with the LPMT and SPMT system.

¹⁶⁵⁷ The resolution and bias of the reconstruction needs to be extremely well characterized: the target resolution of 3% [50] is unprecedented as is required to be able to distinguished between Normal Ordering (NO) and Inverse Ordering (IO). The non-linearity uncertainty needs to be contained under 1% or the risk appear to measure the wrong ordering [27].

¹⁶⁶¹ One of the possible non-linearity source, that will be used as a reference source in this chapter, is the charge non-linearity (QNL) that will be detailed in next section. The dual calorimetry will be able to solve this problem, using calibrations method and measurements that will be used to correct it [27].

¹⁶⁶⁴ More generally, comparing the results of the two system will allow to detect potential issues on the calibration or reconstruction. This is done in this thesis by comparing directly the spectra and oscillation parameters measurements of the two system.

¹⁶⁶⁷ The study of the independents results of the two system can bring some informations [79] but this is missing the important correlation that should be present between the two system: they see the same events, in the same scintillator, their bound to be correlated. We explore in this chapter a preliminary study of the impact of those correlation via multiple methods and the impact of QNL at various degree.

¹⁶⁷² In the next section will discuss the motivations behind this study. In section 7.2, I present the approaches and assumptions in this study. In section 7.3 I present the fit framework used and following in section 7.4 the technical improvement brought and the difficulties faced during the development. To end this chapter I present the results in 7.5 and discuss the conclusion and perspectives in 7.6.

1676 7.1 Motivations

1677 7.1.1 Discrepancies between the SPMT and LPMT results

1678 As discussed in the introduction of this chapter, the SPMT system and the LPMT system will observe
 1679 the same events. This mean that, after calibration, if the two system show significant differences
 1680 in their results this is the signal of potential overlook of an effect or problem. Being able to detect
 1681 such differences is thus crucial as, as discussed above, even the smallest deviation from our model
 1682 could lead to the impossibility to measure the Mass Ordering (MO) or even worse, wrong our
 1683 measurement.

1684 The two system are expected to have the same sensitivity to the oscillation parameters θ_{12} and Δm_{21}^2
 1685 [11]. We will thus rely on the measurement of those two parameters to detect potential discrepancies.

1686 We could just look at the value and compare them to the estimated independent error of the two
 1687 system, but we believe and will demonstrate in this chapter that the independent study of the two
 1688 system is missing a lot of informations, and that, by taking into account the statistic and systematic
 1689 correlations between the two systems, we can produce much more powerful statistical test.

1690 Our work in this chapter is to develop such tools. The first step is, of course, to verify that in the
 1691 case of no discrepancies, the results are coherent with the independent analysis. This will give us
 1692 the distribution of those statistical test in absence of discrepancies. When we will have real data, we
 1693 will be able to compare it to those distribution to obtain a p-value characterizing the absence of those
 1694 potential discrepancies.

1695 To evaluate the power of our methods, we need to simulate a concrete discrepancy. We decide to
 1696 study a plausible effect, the Charge Non-Linearity (QNL) that is detailed next section, but the goal of
 1697 those tools is to be discrepancy agnostic, as those discrepancies could come from a variety of source
 1698 (calibration issue, insufficient simulation tuning, etc...)

1699 7.1.2 Charge Non-Linearity (QNL)

1700 The CD energy response is subject of two kind on non-linearity, the first one is the LS response
 1701 non-linearity where the LS photo-production not linear with the deposited energy as illustrated in
 1702 figure 2.12a. The second one is the LPMT response non-linearity where the charge read from the
 1703 LPMT is not linear in respect to the number of collected Photo-Electron (PE) (see section 2.3).

1704 The LS non-linearity comes from physics sources. Particles interaction in the LS will produce mainly
 1705 scintillation light as discussed in section 2.2.2 but will also produce some cherenkov light (< 10% of
 1706 the collected light). Both mechanisms posses intrinsic non-linearity, for the Cherenkov emission it's
 1707 dependent on the velocity of charged particle velocity while the scintillation photon-yield follow a
 1708 so-called Birk's law with a "quenching" effect depending on the energy and type of particle [16]. This
 1709 results in a channel wise QNL.

1710 The LPMT response non-linearity can come from sheer saturation when subject to a high rate of
 1711 photon inducing a gain non-linearity or come from readout effects such as the electronic noise, the
 1712 overshoot, the integration time window and even the waveform algorithm. All of those effects results
 1713 in a channel wise QNL.

1714 Precedent studies [27] suggest a model to emulate this non-linearity response that will be used in this
 1715 work. We thus define the channel wise non-linearity that would be applied to each LPMT readout

$$\frac{Q_{rec}}{Q_{true}} = \frac{-\gamma_{qnl}}{9} Q_{true} + \frac{\gamma_{qnl} + 9}{9} \quad (7.1)$$

1716 where Q_{rec} is the reconstructed number of PE by the PMT, Q_{true} is true number of PE that hit the
 1717 PMT, and γ_{qnl} is a factor representing the amplitude of the non-linearity.

1718 We also define an event-wise non-linearity characterized by

$$\frac{E_{vis}}{E_{true}} = \frac{-\alpha_{qnl}}{9} E_{true} + \frac{\alpha_{qnl} + 9}{9} \quad (7.2)$$

1719 where E_{vis} is the visible energy that can be collected by the detector and E_{true} is the true deposited
 1720 energy. An example of the effect of such event-wise QNL is presented in figure 7.1.

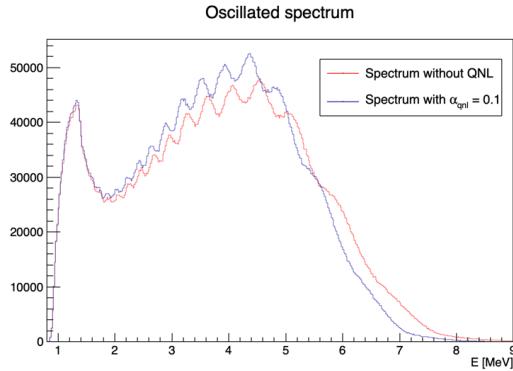


FIGURE 7.1 – Two oscillated spectrums of $1e7$ event expected in JUNO. In red the spectrums without supplementary QNL. In blue the same spectrum but where an event-wise QNL $\alpha_{qnl} = 10\%$ is added.

1721 Using 1M from the JUNO official simulation J23.0.1-rc8.dc1 (released the 7th January 2024), we
 1722 simulated events up to the photon collection in LPMTs and simulated an additional channel-wise
 1723 QNL by applying the equation 7.1 to the number of collected photons.

1724 In figure 7.2a we show the distribution of the ratio $\frac{Q_{rec}}{Q_{true}}$ for central events ($R < 4m$) and different
 1725 value of γ_{qnl} . In figure 7.2a we show the mean of this distribution as function of the energy. We show
 1726 effective α_{qnl} for each value of γ_{qnl} . We see that using the event-wise QNL is equivalent to the mean
 1727 behavior of using channel-wise QNL.

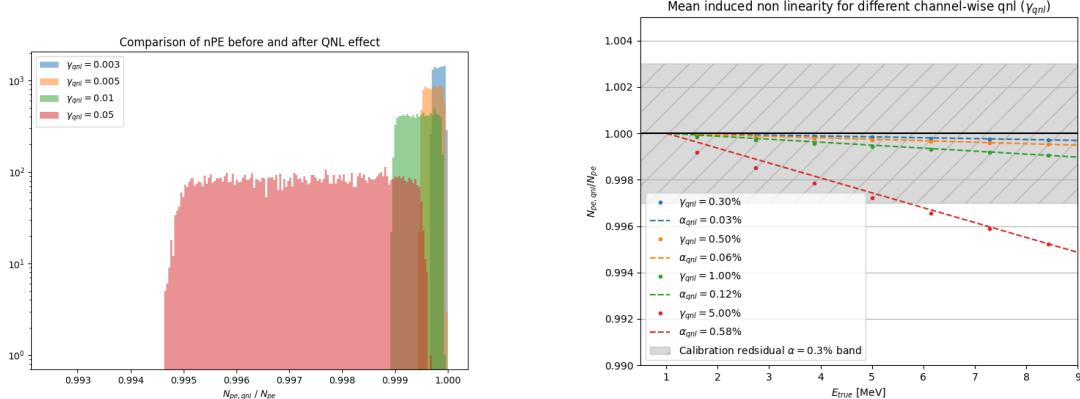
1728 When using channel-wise non-linearity, we need to simulate a number of PE per LPMT, the process
 1729 can be quite tedious if we want a realistic simulation so in this study we are only using event-wise
 1730 non-linearity to make the process simpler. This event-wise non-linearity will be characterized by
 1731 α_{qnl} .

1732 7.2 Approach

1733 In this section we detail the testing procedure behind each of our tools.

1734 7.2.1 Data production

1735 The first step is the generation of data on which we run our tools. In this study we are producing
 1736 monte-carlo toy. In each toy we generate an $\bar{n}\bar{\nu}_e$ energy spectrum coming from the Taishan, Yangjiang
 1737 and Dayabay reactor power plant, the reactor used as source for the NMO analysis. This is the
 1738 starting point of the two observed spectrum, the LPMT and SPMPT spectrum. On those spectrum, we
 1739 add the physics effect such as the LS non-linearity etc... (more details in section 7.3.1). On top on



(A) Distribution of ratio of collected nPE after the additional QNL over the number of nPE that would be collected for different γ_{qnl} . We select event with an interaction radius $R < 4\text{m}$ to not be affected by the non-uniformity.

(B) Ratio of collected nPE after the additional QNL over the number of nPE that would be collected at different energies. We select event with an interaction radius $R < 4\text{m}$ to not be affected by the non-uniformity. The dots represent the mean of the distribution in figure 7.2a and the dashed line are the equivalent event-wise non-linearity from eq 7.2. The hatched zone is the residual non-linearity expected after calibration [29].

FIGURE 7.2

1740 those effect, we apply the reconstruction resolution of each systems to their respective spectra. We
1741 end up with the two LPMT and SPMT spectrum.

1742 We will study the effect of exposure on our methods at different threshold: 100 days, 1 year, 2 year
1743 and finally 6 years which is the nominal data taking period for the NMO analysis.

1744 Those spectra are generated for different QNL, $\alpha_{qnl} = 0$, no spectrum distortion, and for $\alpha_{qnl} \in$
1745 $0.01, 0.005, 0.003, 0.002, 0.001$. As a reminder, the calibration guarantee a residual event-wise non-
1746 linearity $\alpha_{qnl} \leq 0.003$ [29].

The first test does not require any fitting and we are just comparing the LPMT and SPMT spectra using the expected statistical correlation matrix in the case $\alpha_{qnl} = 0$, for details about the generation of this correlation matrix, refer to section 7.5.1. This test is the indicative χ^2 test or χ^2_{ind} test. In this test we produce a χ^2 representing show the incompatibility between the LPMT and SPMT spectra:

$$\Delta_i = h_{L,i} - h_{S,i} \quad (7.3)$$

$$U = AVA^T \quad (7.4)$$

$$\chi^2_{ind} = \vec{\Delta}^T U^{-1} \vec{\Delta} \quad (7.5)$$

1747 Where $h_{L,i}$ and $h_{S,i}$ are the content of the i th bin of the LPMT and SPMT bin respectively. V is the
1748 covariance matrix of the LPMT + SPMT spectrum. A is a transfers matrix such as:

$$A_{ij} = \frac{\partial \Delta_i}{\partial h_j} = \frac{\partial (h_{L,i} - h_{S,i})}{\partial h_j} \quad (7.6)$$

1749 Thus $A_{ij} = 1$ if $i = j$ and $A_{ij} = -1$ if j is the SPMT bin corresponding to the i LPMT bin.

1750 This χ^2_{ind} is minimal when the statistic between the bins of the LPMT and SPMT spectra follow the

1751 covariance matrix V . By looking at the distribution of this χ^2_{ind} when $\alpha_{qnl} = 0$ we can produce
1752 p-values for the values found when $\alpha_{qnl} \neq 0$.

1753 **7.2.2 Individual fits**

1754 Each of the spectra, LPMT and SPMT, are then fitted individually with and without

1755 **7.3 Fit framework**

1756 **7.3.1 IBD generator**

1757 **7.4 Technical challenges**

1758 **7.5 Results**

1759 **7.5.1 Covariance matrix**

1760 **7.6 Conclusion and perspectives**

¹⁷⁶¹ Chapter 8

¹⁷⁶² Conclusion

¹⁷⁶³ **Appendix A**

¹⁷⁶⁴ **Calculation of optimal α for estimator combination**

¹⁷⁶⁶ This annex the details of the determination of the optimal α for estimator combination presented in
¹⁷⁶⁷ section 4.4.2.

¹⁷⁶⁸ As a reminder, the combined estimator $\hat{\theta}$ of X is defined as

$$\hat{\theta}(X) = \alpha\theta_N + (1 - \alpha)\theta_C; \alpha \in [0; 1] \quad (\text{A.1})$$

¹⁷⁶⁹ where θ_N and θ_C are both estimator of X .

¹⁷⁷⁰ **A.1 Unbiased estimator**

For the unbiased estimator, it is straight-forward. We search α such as $E[\hat{\theta}] = X$

$$E[\hat{\theta}] = E[\alpha\theta_N + (1 - \alpha)\theta_C] \quad (\text{A.2})$$

$$= E[\alpha\theta_N] + E[(1 - \alpha)\theta_C] \quad (\text{A.3})$$

$$= \alpha E[\theta_N] + (1 - \alpha)E[\theta_C] \quad (\text{A.4})$$

$$= \alpha(\mu_N + X) + (1 - \alpha)(\mu_C + X) \quad (\text{A.5})$$

$$X = \alpha\mu_N + \mu_C - \alpha\mu_C + X \quad (\text{A.6})$$

$$0 = \alpha(\mu_N - \mu_C) + \mu_C \quad (\text{A.7})$$

$$(A.8)$$

$$\Rightarrow \alpha = \frac{\mu_C}{\mu_C - \mu_N} \quad (\text{A.9})$$

¹⁷⁷¹ **A.2 Optimal variance estimator**

The α for this estimator is a bit more tricky. By expanding the variance we get

$$\text{Var}[\hat{\theta}] = \text{Var}[\alpha\theta_N + (1 - \alpha)\theta_C] \quad (\text{A.10})$$

$$= \text{Var}[\alpha\theta_N] + \text{Var}[(1 - \alpha)\theta_C] + \text{Cov}[\alpha(1 - \alpha)\theta_N\theta_C] \quad (\text{A.11})$$

$$= \alpha^2\sigma_N^2 + (1 - \alpha)^2\sigma_C^2 + 2\alpha(1 - \alpha)\sigma_N\sigma_C\rho_{NC} \quad (\text{A.12})$$

¹⁷⁷² where, as a reminder, ρ_{NC} is the correlation factor between θ_C and θ_N .

Now we try to find the minima of $\text{Var}[\hat{\theta}]$ with respect to α . For this we evaluate the derivative

$$\frac{d}{d\alpha} \text{Var}[\hat{\theta}] = 2\alpha\sigma_N^2 - 2(1-\alpha)\sigma_C^2 + 2\sigma_N\sigma_C\rho_{NC}(1-2\alpha) \quad (\text{A.13})$$

$$= 2\alpha(\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC}) - 2\sigma_C^2 + 2\sigma_N\sigma_C\rho_{NC} \quad (\text{A.14})$$

then find the minima and maxima of this derivative by evaluating

$$\frac{d}{d\alpha} \text{Var}[\hat{\theta}] = 0 \quad (\text{A.15})$$

$$2\alpha(\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC}) - 2\sigma_C^2 + 2\sigma_N\sigma_C\rho_{NC} = 0 \quad (\text{A.16})$$

$$2\alpha(\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC}) = 2\sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC} \quad (\text{A.17})$$

$$\alpha = \frac{\sigma_C^2 - \sigma_N\sigma_C\rho_{NC}}{\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC}} \quad (\text{A.18})$$

1773 This equation shows only one solution which is a minima. From Eq. A.18 arise two singularities:

1774 — $\sigma_N = \sigma_C = 0$. This is not a problem because as physicists we never measure with an absolute

1775 precision, neither us or our detectors are perfect.

1776 — $\sigma_N = \sigma_C$ and $\rho_{CN} = 1$. In this case θ_C and θ_N are the same estimator in term of variance thus

1777 any value for α yield the same result: an estimator with the same variance as the original ones.

¹⁷⁷⁸ **Appendix B**

¹⁷⁷⁹ **Charge spherical harmonics analysis**

¹⁷⁸⁰ When looking at JUNO events we can clearly see some pattern in the charge repartition based on
¹⁷⁸¹ the event radius as illustrated in figure B.4. When dealing with identifying features and pattern on a
¹⁷⁸² spherical plane, the astrophysics community have been using, with success, the spherical harmonic
¹⁷⁸³ decomposition. The principle is similar to a frequency analysis via Fourier transform. It comes to
¹⁷⁸⁴ saying that a function $f(r, \theta, \phi)$, here our charge repartition of the spherical plane constructed by our
¹⁷⁸⁵ PMTs, can be expressed

$$f(r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l a_l^m r^l Y_l^m(\theta, \phi) \quad (\text{B.1})$$

¹⁷⁸⁶ where a_l^m are constants complex factor, $Y_l^m(\theta, \phi) = Ne^{im\phi} P_l^m(\cos \theta)$ are the spherical harmonics of
¹⁷⁸⁷ degree l and order m and P_l^m their associated Legendre Polynomials. Those harmonics are illustrated
¹⁷⁸⁸ in figure B.1. By reducing the problem to the unit sphere $r = 1$, we get rid of the term r^l . The Healpix
¹⁷⁸⁹ library [76] offer function to efficiently find the a_l^m factor from a given Healpix map.

¹⁷⁹⁰ For the above decomposition, we will define the *Power* of an harmonic as

$$S_{ff}(l) = \frac{1}{2l+1} \sum_{m=-l}^l |a_l^m|^2 \quad (\text{B.2})$$

¹⁷⁹¹ and the *Relative Power* as:

$$P_l^h = \frac{S_{ff}(l)}{\sum_l S_{ff}(l)} \quad (\text{B.3})$$

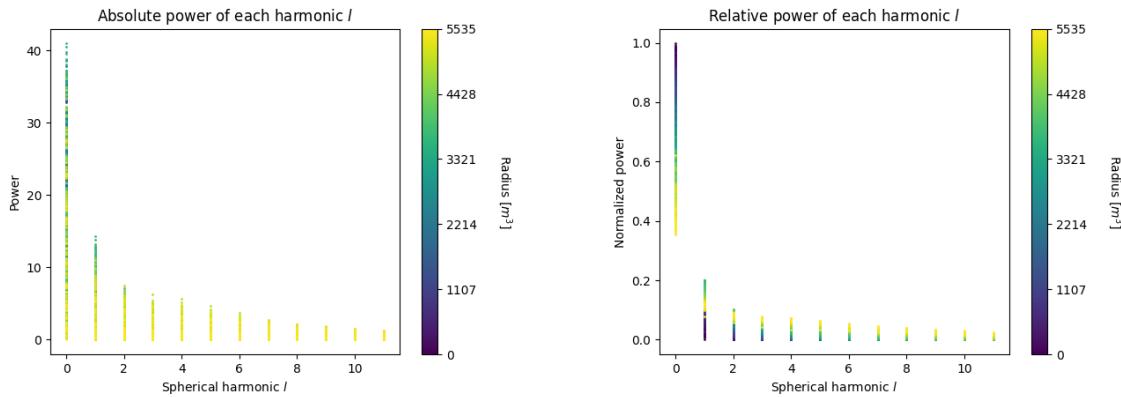
¹⁷⁹² For this study we will use 10k positron events with $E_{kin} \in [0; 9]$ MeV uniformly distributed in the
¹⁷⁹³ CD from the JUNO official simulation version J23.0.1-rc8.dc1 (released the 7th January 2024). All the
¹⁷⁹⁴ event are *calib* level, with simulation of the physics, electronics, digitizations and triggers. We first
¹⁷⁹⁵ take a sub-set of 1k events and look at the power and relative power distribution depending on the
¹⁷⁹⁶ radius and harmonic degree l . The results are shown in figure B.2. While don't see any pattern in
¹⁷⁹⁷ absolute power, it is pretty clear that there is a correlation between the relative power of $l = 0$ and
¹⁷⁹⁸ the radius of the event.

¹⁷⁹⁹ When applying the same study but dependent on the energy, no clear correlation appear. The results
¹⁸⁰⁰ for the $l = 0$ harmonic are presented in the figure B.5. Thus, in this study we will focus on the radial
¹⁸⁰¹ dependency of the relative power of each harmonic.

¹⁸⁰² In figures B.6 and B.7 are presented the distribution of the relative power of each harmonic for $l \in$
¹⁸⁰³ $[0, 11]$. The relation between the radius and the relative power become even more clear, especially
¹⁸⁰⁴ for the first harmonics $l \in [0, 4]$. After that for $l > 4$ their relative power is close to 0 for central event,
¹⁸⁰⁵ thus loosing power. It also interesting to note the change of behavior in the TR area, clearly visible
¹⁸⁰⁶ for $l = 1$ and $l = 2$.

$l:$		$P_\ell^m(\cos \theta) \cos(m\varphi)$	$P_\ell^{ m }(\cos \theta) \sin(m \varphi)$	
0	s			
1	p			
2	d			
3	f			
4	g			
5	h			
6	i			
m:	6 5 4 3 2 1 0	-1 -2 -3 -4 -5 -6		

FIGURE B.1 – Illustration of the real part of the spherical harmonics

FIGURE B.2 – Scatter plot of the absolute and relative power, respectively on the left and right plot, of each harmonic degree l . The color indicate the radius of the event.

1807 As an erzats of reconstruction algorithm, we fit each of those distribution with a 9th degree polynomial
 1808 which give us the relation

$$F(R^3) \longmapsto P_l^h \quad (\text{B.4})$$

1809 We do it this way because some of the distribution have multiple solution for a given relative power,
 1810 for example $l = 1$, while each radius give only one power. We now just need to find

$$F^{-1}(P_l^h) \longmapsto R^3 \quad (\text{B.5})$$

1811 Inverting a 9th degree polynomial is hard, if not impossible. The presence of multiple roots for the
 1812 same power complexify the task even more. To circumvent this problem, we reconstruct the radius
 1813 by locating the minima of $(F(R^3) - \hat{P}_l^h)^2$ where \hat{P}_l^h is the measured power fraction.

1814 To distinguish between multiple possible minima, we use as a starting point the radius given by the
 1815 procedure on $l = 0$ that, by looking at the fit in figure B.6, should only present one minima. For $l > 0$
 1816 we also impose bound on the possible reconstructed R^3 as $R^3 \in [R_0^3 - 100, R_0^3 + 100]$ where R_0^3 is the
 1817 reconstructed R^3 by the harmonic $l = 0$.

1818 The minimization algorithm used are the Bent algorithm for $l = 0$ and the Bounded algorithm for
 1819 $l > 0$ provided by the Scipy library [80]. We then do the mean of the reconstructed radius from
 1820 the different harmonics. The reconstruction results are shown in figure B.3. The performance seems
 1821 correct but we see heavy fluctuation in the bias. To really be used as a reconstruction algorithm, the
 1822 method needs to be refined as discussed in the next section.

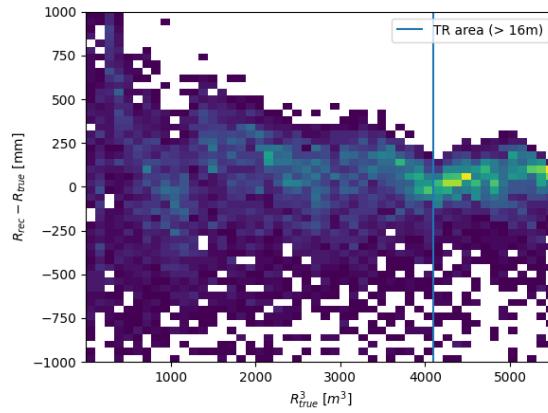


FIGURE B.3 – Error on the reconstructed radius vs the true radius by the harmonic method

1823 Conclusion

1824 We have clearly shown in this analysis the relevance the of relative harmonic power for radius
 1825 reconstruction, and provided an erzats of a reconstruction algorithm. We will not delve further in
 1826 this thesis but if we wanted to refine this algorithm multiple paths can be explored:

- 1827 — No energy signature in the harmonics: This is surprising that there is no correlation between
 1828 the energy and the amplitude of the harmonics. We know that the energy is heavily correlated
 1829 with the total number of photoelectrons collected, it would be unintuitive that we see no
 1830 relation.
- 1831 — Localization of the event: We shown here the relation between the relative power of the har-
 1832 monic and the radius but don't get any information about the θ and ϕ spherical coordinates.
 1833 This information is probably hidden in the individual power of each order m of the degree l .
 1834 This intuition comes from the figure B.1 where in the higher degree l we see that the order m
 1835 are oriented. Intuitively, the order should be able to indicate a direction where the signal is
 1836 more powerful.
- 1837 — Combination of the degree power: Here we combined the radius reconstructed by the dif-
 1838 ferent degree via a simple mean but we shown in section 4.4.2 and annex A that this is note
 1839 the optimal way to combine estimator. A more refined algorithm probably exist to take into
 1840 account the predicting power of each order.

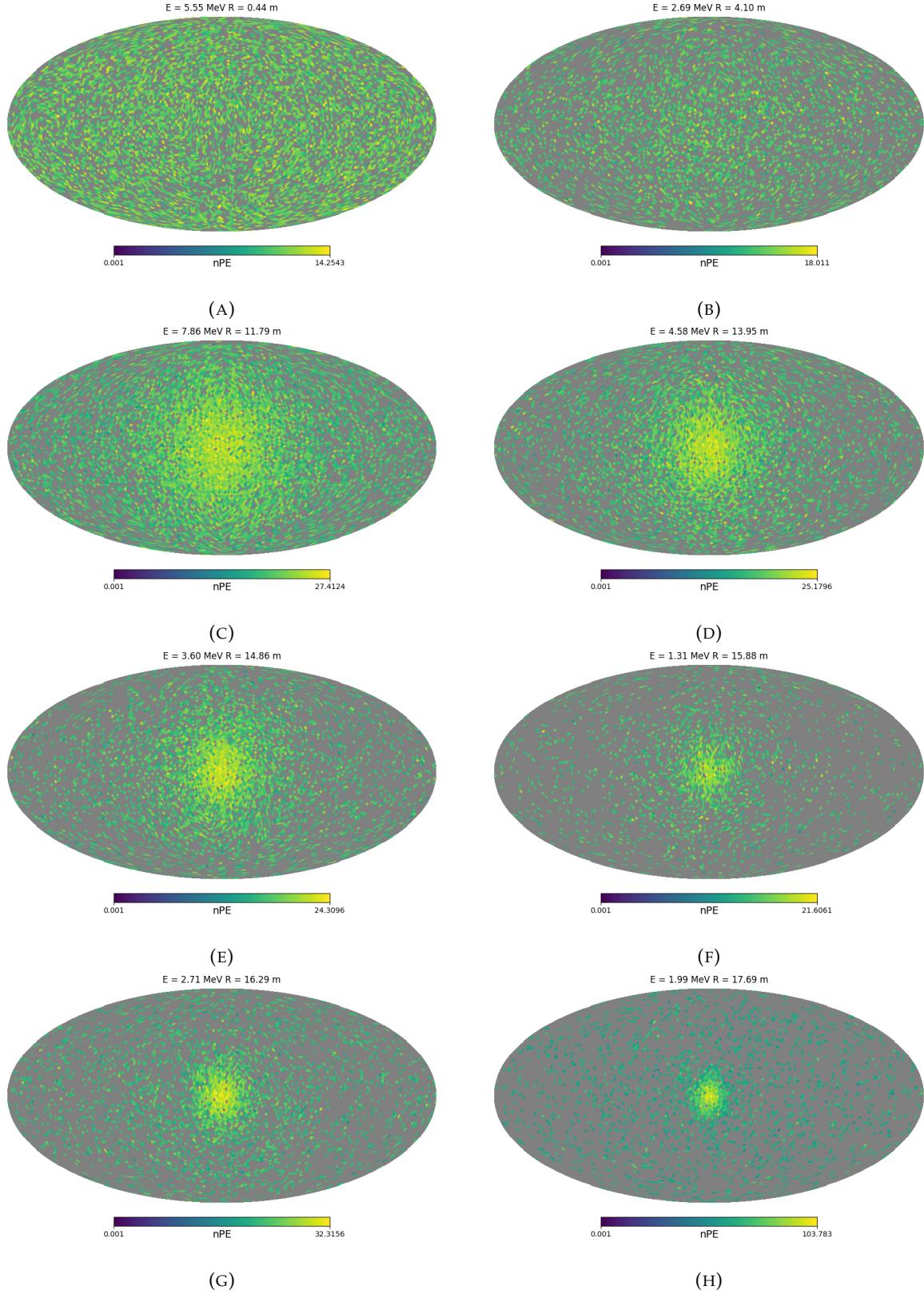


FIGURE B.4 – Charge repartition in JUNO as seen by the Healpix segmentation. Those are Healpix map of order 5 (i.e. 12288 pixels). The color represent the summed charge of the PMTs in each pixels. The color scale is logarithmic. The view have been centered to prevent event deformations.

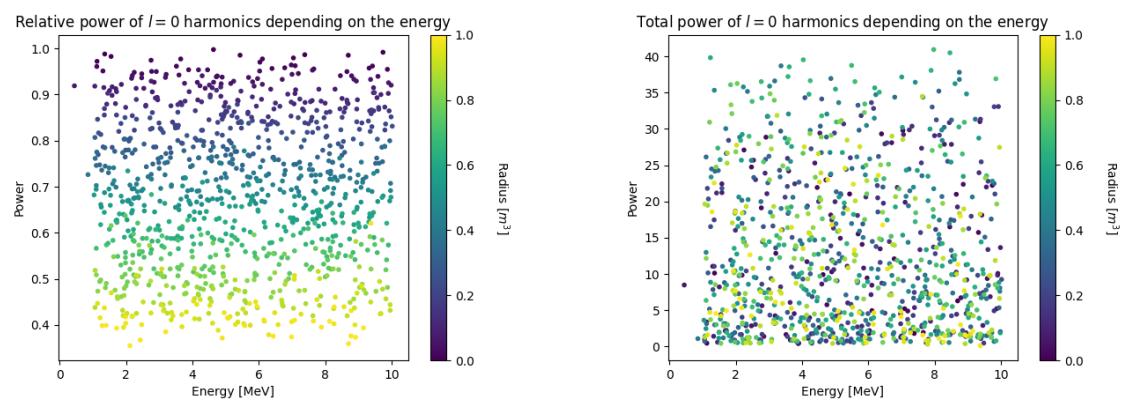


FIGURE B.5 – Scatter plot of the absolute and relative power, respectively on the left and right plot, of the $l = 0$ harmonic. The color indicate the radius of the event.

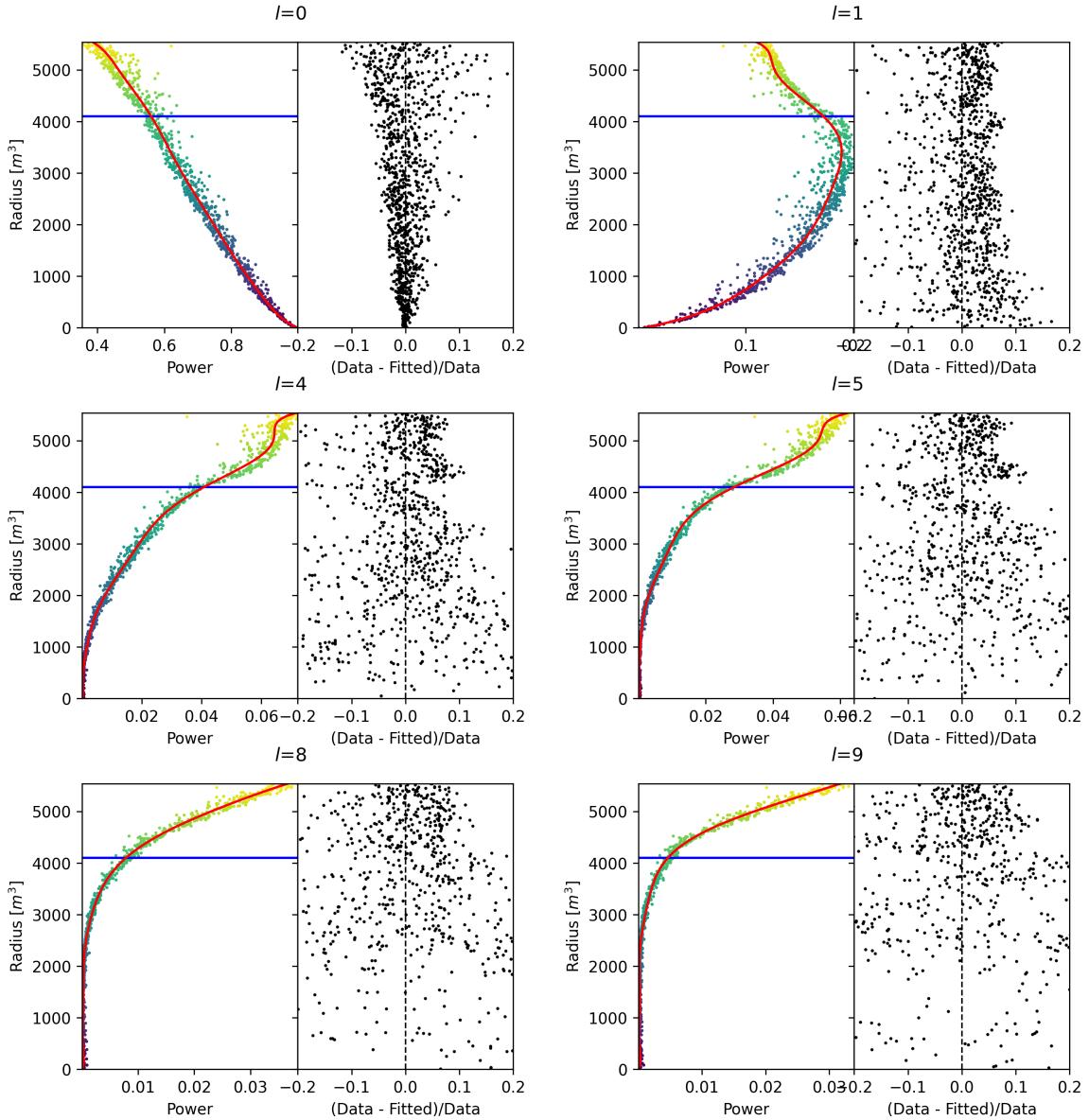


FIGURE B.6 – Plot of the distribution of the relative power of each harmonic dependent on R^3 (on the left). The Total Reflection (TR) area is represented by the horizontal blue line. The distribution are fitted using a 9th degree polynomial (red curve). The relative power error between the distribution and the fit is represented on the left. **Part 1**

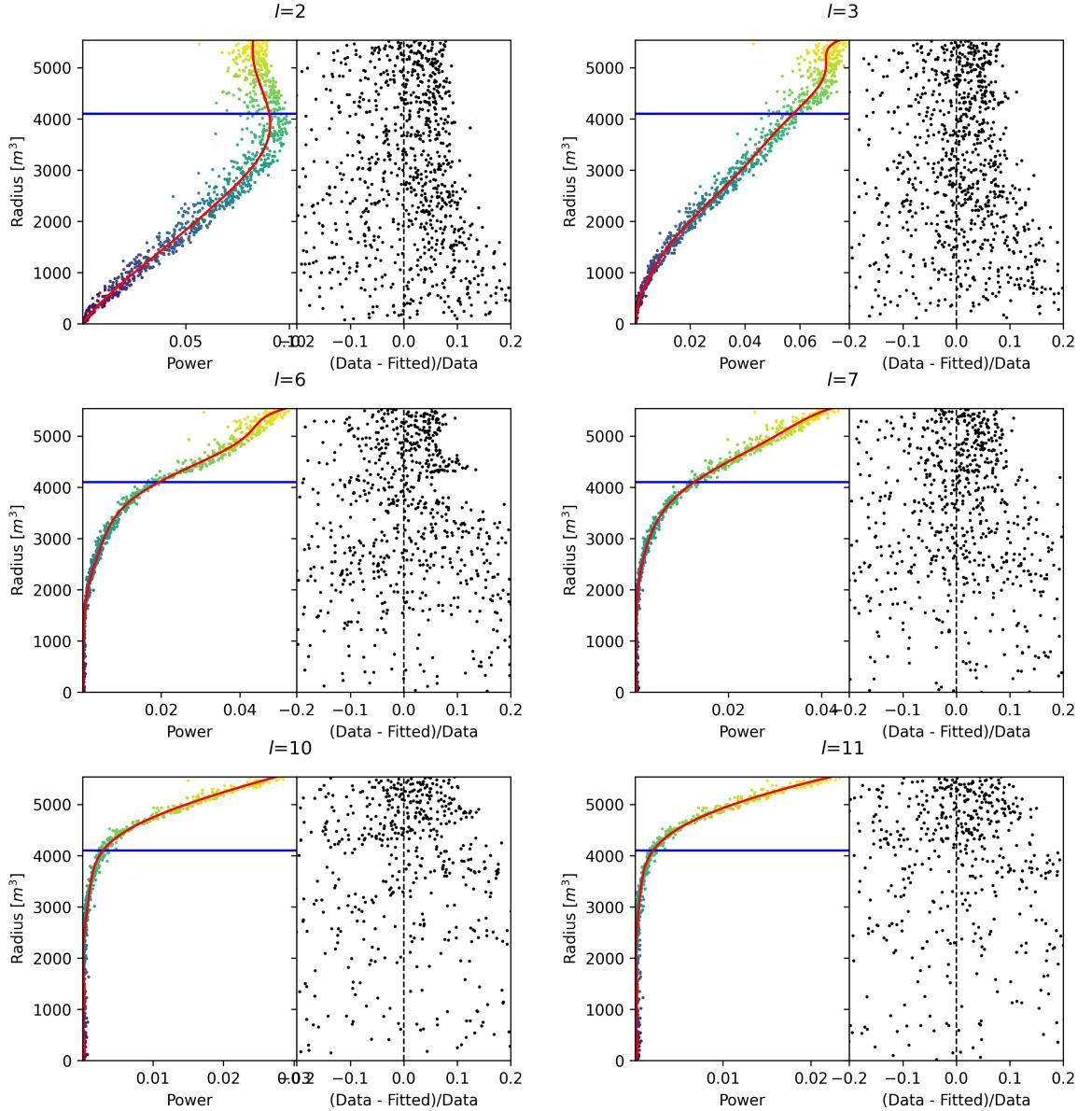


FIGURE B.7 – Plot of the distribution of the relative power of each harmonic dependent on R^3 (on the left). The Total Reflection (TR) area is represented by the horizontal blue line. The distribution are fitted using a 9th degree polynomial (red curve). The relative power error between the distribution and the fit is represented on the left. **Part 2**

List of Tables

1842	2.1	Characteristics of the nuclear power plants observed by JUNO. The IBD rate are estimated from the baselines, the reactors full thermal power, selection efficiency and the current knowledge of the oscillation parameters	13
1843	2.2	A summary of precision levels for the oscillation parameters. The reference value (PDG 2020 [16]) is compared with 100 days, 6 years and 20 years of JUNO data taking.	15
1844	2.3	Detectable neutrino signal in JUNO and the expected signal rates and major background sources	15
1845	2.4	List of sources and their process considered for the energy scale calibration	23
1846	2.5	Calibration program of the JUNO experiment	25
1847	2.6	Features used by the BDT for vertex reconstruction	36
1848	2.7	Features used by the BDTE algorithm. <i>pe</i> and <i>ht</i> reference the charge and hit-time distribution respectively and the percentages are the quantiles of those distributions. <i>cht</i> and <i>cc</i> reference the barycenters of hit time and charge respectively	36
1849	4.1	Sets of hyperparameters values considered in this study	56
1850	5.1	Parameters of the 5th degree polynomial used to correct Omilrec reconstructed energy.	77
1851			
1852			
1853			
1854			
1855			
1856			

List of Figures

1857	2.1 On the left: Location of the JUNO experiment and its reactor sources in southern china. On the right: Aerial view of the experimental site	11
1859	2.2 Expected number of neutrinos event per MeV in JUNO after 6 years of data taking. The black curve shows the flux if there was no oscillation. The light gray curve shows the oscillation if only the solar terms are taken in account (θ_{12} , Δm_{21}^2). The blue and red curve shows the spectrum in the case of, respectively, NO and IO. The dependency of the oscillation to the different parameters are schematized by the double sided arrows. We can see the NMO sensitivity by looking at the fine phase shift between the red and the blue curve.	12
1860		
1861		
1862		
1863		
1864		
1865		
1866		
1867		
1868		
1869		
1870	2.3 Expected visible energy spectrum measured with the LPMT system with (grey) and without (black) backgrounds. The background amount for about 7% of the IBD candidate and are mostly localized below 3 MeV [11]	14
1871		
1872		
1873	2.4	17
1874	a Schematics view of the JUNO detector.	17
1875	b Top down view of the JUNO detector under construction	17
1876		
1877	2.5 Schematics of an IBD interaction in the central detector of JUNO	18
1878		
1879	2.6 Schematics of the supporting node for the acrylic vessel	19
1880		
1881	2.7 On the left: Quantum efficiency (QE) and emission spectrum of the LAB and the bis-MSB [20]. On the right: Sensitivity of the Hamamatsu LPMT depending on the wavelength of the incident photons [22].	19
1882		
1883	2.8 Schematic of a PMT	20
1884		
1885	2.9 The LPMT electronics scheme. It is composed of two part, the <i>wet</i> electronics on the left, located underwater and the <i>dry</i> electronics on the right. They are connected by Ethernet cable for data transmission and a dedicated low impedance cable for power distribution	21
1886		
1887	2.10 Schematic of the JUNO SPMT electronic system (left), and exploded view of the main component of the UWB (right)	22
1888		
1889	2.11 The JUNO top tracker	23
1890		
1891	2.12 Fitted and simulated non linearity of gamma, electron sources and from the ^{12}B spectrum. Black points are simulated data. Red curves are the best fits. Figures taken from [29].	24
1892		
1893	a Gamma non-linearity	24
1894	b Boron spectrum	24
1895	c Electron non-linearity	24
1896		
1897	2.13 Overview of the calibration system	25
1898		
1899	2.14 Event-level instrumental non-linearity, defined as the ratio of the total measured LPMT charge to the true charge for events uniformly distributed in the detector. The solid red line represents event-level non-linearity without the channel-level correction, with position non-uniformity obtained at 1 MeV applied, in an extreme hypothetical scenario of 50% non-linearity over 100 PEs for the LPMTs. The dashed blue line represents that after the channel-level correction. The gray band shows the residual uncertainty of 0.3%, after the channel-level correction. Figure taken from [29].	26
1900		
	2.15	27

1901	a	Schematic of the TAO satellite detector	27
1902	b	Schematic of the OSIRIS satellite detector	27
1903	2.16	.	29
1904	a	Illustration of the different optical photons reflection scenarios. 1 is the reflection of the photon at the interface LS-acrylic or acrylic-water. 2 is the transmission of the photons through the interfaces. 3 is the conduction of the photon in the acrylic.	29
1905	b	Heatmap of R_{rec} and $R_{rec} - R_{true}$ as a function of R_{true} for 4MeV prompt signals uniformly distributed in the detector calculated by the charge based algorithm	29
1906	2.17	.	30
1907	a	Δt distribution at different iterations step j	30
1908	b	Heatmap of R_{rec} and $R_{rec} - R_{true}$ as a function of R_{true} for 4MeV prompt signals uniformly distributed in the detector calculated by the time based algorithm	30
1909	2.18	Bias of the reconstructed radius R (left), θ (middle) and ϕ (right) for multiple energies by the time likelihood algorithm	31
1910	2.19	On the left: Resolution of the reconstructed R as a function of the energy in the TR area ($R^3 > 4000\text{m}^3 \equiv R > 16\text{m}$) by the charge and time likelihood algorithms. On the right: Bias of the reconstructed R in the TR area for different energies by the charge likelihood algorithm	32
1911	2.20	Radial resolution of the different vertex reconstruction algorithms as a function of the energy	32
1912	2.21	.	33
1913	a	Spherical coordinate system used in JUNO for reconstruction	33
1914	b	Definition of the variables used in the energy reconstruction	33
1915	2.22	.	35
1916	a	Radial resolutions of the likelihood-based algorithm TMLE, QMLE and QTMLE	35
1917	b	Energy resolution of QMLE and QTMLE using different vertex resolutions	35
1918	2.23	Projection of the LPMTs in JUNO on a 2D plane. (a) Show the distribution of all PMTs and (b) and (c) are example of what the charge and time channel looks like respectively	37
1919	2.24	Radial (left) and energy (right) resolutions of different ML algorithms. The results presented here are from [42]. DNN is a deep neural network, BDT is a BDT, ResNet-J and VGG-J are CNN and GNN-J is a GNN.	38
1920	3.1	Example of a BDT that determine if the given object is a duck	42
1921	3.2	.	44
1922	a	Schema of a FCDNN	44
1923	b	Illustration of a composition of ReLU matching a function	44
1924	3.3	Illustration of the effect of a convolution filter. Here we apply a filter with the aim do detect left edges. We see in the resulting image that the left edges of the duck are bright yellow where the right edges are dark blue indicating the contour of the object. The convolution was calculated using [58].	44
1925	3.4	.	45
1926	a	Example of images in the MNIST dataset	45
1927	b	Schema of the CNN used in Pytorch example to process the MNIST dataset	45
1928	3.5	.	48
1929	a	Illustration of SGD falling into a local minima	48
1930	b	Illustration of the Adam momentum allowing it to overcome local minima	48
1931	3.6	Illustration of the SGD optimizer. In blue is the value of the loss function, orange, green and red are the path taken by the optimized parameter during the training for different LR.	48
1932	a	Illustration of the SGD optimizer on one parameter θ on the MAE Loss. We see here that it has trouble reaching the minima due to the gradient being constant.	48

1952	b	Illustration of the SGD optimizer on one parameter θ on the MAE Loss. We see two different behavior: A smooth one (orange and red) when the LR is small enough and a more chaotic one when the LR is too high.	48
1953			49
1954			
1955	3.7	
1956	a	Illustration of overtraining. The task at hand is to determine depending on two input variable x and y if the data belong to the dataset A or the dataset B . The expected boundary between the two dataset is represented in grey. A possible boundary learnt by overtraining is represented in brown.	49
1957			49
1958	b	Illustration of a very simple NN	49
1959			49
1960	3.8	Illustration of the ResNet framework	50
1961			
1962	3.9	Illustration of the gradient explosion. Here it can be solved with a lower learning rate but its not always the case.	51
1963			
1964	4.1	Graphic representation of the VGG-16 architecture, presenting the different kind of layer composing the architecture.	54
1965			
1966	4.2	Repartition of SPMTs in the image projection. The color scale is the number of SPMTs per pixel	58
1967			
1968	4.3	Example of a high energy, radial event. We see a concentration of the charge on the bottom right of the image, clear indication of a high radius event. On the left: the charge channel. The color is the charge in each pixel in NPE equivalent. On the right: The time channel in nanoseconds.	59
1969			
1970	4.4	Example of a low energy, radial event. The signal here is way less explicit, we can kind of guess that the event is located in the top middle of the image. On the left: the charge channel. The color is the charge in each pixel in NPE equivalent. On the right: The time channel in nanoseconds.	59
1971			
1972	4.5	Example of a high energy, central event. In this image we can see a lot of signal but uniformly spread, this is indicative of a central event. On the left: the charge channel. The color is the charge in each pixel in NPE equivalent. On the right: The time channel in nanoseconds.	60
1973			
1974	4.6	Example of a low energy, central event. Here there is no clear signal, the uniformity of the distribution should make it central. On the left: the charge channel. The color is the charge in each pixel in NPE equivalent. On the right: The time channel in nanoseconds.	60
1975			
1976	4.7	61
1977	a	Distribution of PE/MeV in the J23 Dataset. This distribution is profiled and fitted using equation 4.6	61
1978	b	On top: Distribution of PE vs Energy. On bottom: Using the values extracted in 4.7a, we calculate the ration signal over background + signal	61
1979			
1980	4.8	Reconstruction performance of the “gen_30” model on J21 data and it’s comparison to the performances of the classic algorithm “Classical algorithm” from [66]. The top part of each plot is the resolution and the bottom part is the bias.	63
1981	a	Resolution and bias of energy reconstruction vs energy	63
1982	b	Resolution and bias of energy reconstruction vs radius	63
1983	c	Resolution and bias of radius reconstruction vs energy	63
1984	d	Resolution and bias of radius reconstruction vs radius	63
1985	e	Resolution and bias of radius reconstruction vs θ	63
1986	f	Resolution and bias of radius reconstruction vs ϕ	63
1987			
1988	4.9	Error distribution of the different component of the vertex by “gen_30”. The reconstructed component are x , y and z but we see similar behavior in the error of R , θ and ϕ	64
1989	a	Distribution of the error on reconstructed x by “gen_30”	64
1990	b	Distribution of the error on reconstructed y by “gen_30”	64
1991	c	Distribution of the error on reconstructed z by “gen_30”	64

2004	d	Distribution of the error on reconstructed R by "gen_30"	64
2005	e	Distribution of the error on reconstructed θ by "gen_30"	64
2006	f	Distribution of the error on reconstructed ϕ by "gen_30"	64
2007	4.10	65
2008	a	Distribution of "gen_30" reconstructed energy and true energy of the analysis dataset (J21)	65
2009	b	Distribution of "gen_42" reconstructed energy and true energy of the analysis dataset (J23)	65
2010	4.11	Radius bias (on the left) and resolution(on the right) of the classical algorithm in a E, R^3 grid	65
2011	4.12	Reconstruction performance of the "gen_30" model on J21, the classic algorithm "Classical algorithm" from [66] and the combination of both using weighted mean. The top part of each plot is the resolution and the bottom part is the bias.	66
2012	a	Resolution and bias of energy reconstruction vs energy	66
2013	b	Resolution and bias of energy reconstruction vs radius	66
2014	c	Resolution and bias of radius reconstruction vs energy	66
2015	d	Resolution and bias of radius reconstruction vs radius	66
2016	e	Resolution and bias of radius reconstruction vs θ	66
2017	f	Resolution and bias of radius reconstruction vs ϕ	66
2018	4.13	Correlation between CNN and classical method reconstruction (on the left) for energy and (on the right) for radius in a E, R^3 grid	67
2019	4.14	Reconstruction performance of the "gen_42" model on J23 data and it's comparison to the performances of the classic algorithm "Classical algorithm" from [66]. The top part of each plot is the resolution and the bottom part is the bias.	68
2020	a	Resolution and bias of energy reconstruction vs energy	68
2021	b	Resolution and bias of energy reconstruction vs radius	68
2022	c	Resolution and bias of radius reconstruction vs energy	68
2023	d	Resolution and bias of radius reconstruction vs radius	68
2024	e	Resolution and bias of radius reconstruction vs θ	68
2025	f	Resolution and bias of radius reconstruction vs ϕ	68
2026	5.1	71
2027	a	Illustration of the different nodes in our graphs and their relations.	71
2028	b	Illustration of what a dense adjacency matrix would looks like and the part we are really interested in. Because Fired \rightarrow Mesh and Mesh \rightarrow I/O relations are undirected, we only consider in practice the top right part of the matrix for those relations.	71
2029	5.2	Illustration of the healpix segmentation. On the left: A segmentation of order 0. On the right: A segmentation of order 1	71
2030	5.3	Features held by the nodes and edges in the graph. $D_{m_1 \rightarrow m_2}^{-1}$ is the inverse of the distance between two mesh center. The features P_I^h , \mathbb{A} and \mathbb{B} are detailed in section 5.2	72
2031	5.4	Illustration of the different update function needed by our GNN	73
2032	5.5	Distribution of the number of hits depending on the energy. On the right: for the LPMT system. In the middle : for the SPMT system. On the left: For both system.	74
2033	a	74
2034	b	74
2035	c	74
2036	5.6	Distribution of the number of hits depending on the radius. On the right: for the LPMT system. On the right : for the SPMT system. To prevent the superposition of structure of different scales we limit ourselves to the energy range $E_{true} \in [0, 9]$	75
2037	a	75
2038	b	75

2055	5.7	Schema of the JWGv8.4.0 architecture, the colored triplet is the graph configuration after each JWG layers	76
2056	5.8	Comparison between Omilrec E_{rec} and the true energy E_{true} . The profile of the distribution E_{true}/E_{rec} vs E_{rec} is fitted with a 5th degree polynomial.	78
2057	5.9	Reconstruction performance of the Omilrec algorithm based on QTMLE presented in section 2.6, JWGv8.4 presented in this chapter and the combination between the two as presented in section 4.4.2. The top part of each plot is the resolution and the bottom part is the bias.	79
2058	a	Resolution and bias of energy reconstruction vs energy	79
2059	b	Resolution and bias of energy reconstruction vs radius	79
2060	c	Resolution and bias of radius reconstruction vs energy	79
2061	d	Resolution and bias of radius reconstruction vs radius	79
2062	e	Resolution and bias of radius reconstruction vs θ	79
2063	f	Resolution and bias of radius reconstruction vs ϕ	79
2064			
2065	7.1	Two oscillated spectrums of $1e7$ event expected in JUNO. In red the spectrums without supplementary QNL. In blue the same spectrum but where an event-wise QNL $\alpha_{qnl} = 10\%$ is added.	85
2066	7.2	86
2067	a	Distribution of ratio of collected nPE after the additional QNL over the number of nPE that would be collected for different γ_{qnl} . We select event with an interaction radius $R < 4m$ to not be affected by the non-uniformity.	86
2068	b	Ratio of collected nPE after the additional QNL over the number of nPE that would be collected at different energies. We select event with an interaction radius $R < 4m$ to not be affected by the non-uniformity. The dots represent the mean of the distribution in figure 7.2a and the dashed line are the equivalent event-wise non-linearity from eq 7.2. The hatched zone is the residual non-linearity expected after calibration [29].	86
2069			
2070	B.1	Illustration of the real part of the spherical harmonics	94
2071	B.2	Scatter plot of the absolute and relative power, respectively on the left and right plot, of each harmonic degree l . The color indicate the radius of the event.	94
2072	B.3	Error on the reconstructed radius vs the true radius by the harmonic method	95
2073	B.4	Charge repartition in JUNO as seen by the Healpix segmentation. Those are Healpix map of order 5 (i.e. 12288 pixels). The color represent the summed charge of the PMTs in each pixels. The color scale is logarithmic. The view have been centered to prevent event deformations.	96
2074	a	96
2075	b	96
2076	c	96
2077	d	96
2078	e	96
2079	f	96
2080	g	96
2081	h	96
2082	B.5	Scatter plot of the absolute and relative power, respectively on the left and right plot, of the $l = 0$ harmonic. The color indicate the radius of the event.	97
2083	B.6	Plot of the distribution of the relative power of each harmonic dependent on R^3 (on the left). The Total Reflection (TR) area is represented by the horizontal blue line. The distribution are fitted using a 9th degree polynomial (red curve). The relative power error between the distribution and the fit is represented on the left. Part 1	98

- 2104 B.7 Plot of the distribution of the relative power of each harmonic dependent on R^3 (on
2105 the left). The Total Reflection (TR) area is represented by the horizontal blue line. The
2106 distribution are fitted using a 9th degree polynomial (red curve). The relative power
2107 error between the distribution and the fit is represented on the left. **Part 2** 99

²¹⁰⁸ List of Abbreviations

ACU	Automatic Calibration Unit
BDT	Boosted Decision Tree
CD	Central Detector
CLS	Cable Loop System
CNN	Convolutional NN
DNN	Deep NN
DN	Dark Noise
EDM	Event Data Model
FCDNN	Fully Connected Deep NN
GNN	Graph NN
GT	Guiding Tube
IBD	Inverse Beta Decay
IO	Inverse Ordering
JUNO	Jiangmen Underground Neutrino Observatory
LPMT	Large PMT
LR	Learning Rate
LS	Liquid Scintillator
MC	Monte Carlo simulation
ML	Machine Learning
MSE	Mean Squared Error
NMO	Neutrino Mass Ordering
NN	Neural Network
NO	Normal Ordering
NPE	Number of Photo Electron
OSIRIS	Online Scintillator Internal Radioactivity Investigation System
PE	Photo Electron
PMT	Photo-Multipliers Tubes
PRelu	Parametrized Rectified Linear Unit
QNL	Charge (Q) Non Linearity
ROV	Remotely Operated under-LS Vehicle
ReLU	Rectified Linear Unit
ResNet	Residual Network
SGD	Stochastic Gradient Descent
SPMT	Small PMT
TAO	Taishan Antineutrino Oservatory
TR Area	Total Reflexion Area
TTS	Time Transit Spread
TT	Top Tracker
UWB	Under Water Boxes
WCD	Water Cherenkov Detector

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