



Enhancing Event Reconstruction with Machine Learning for Water Cherenkov Detectors of Hyper-Kamiokande

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## **The Hyper-Kamiokande Experiment**

**Hyper-Kamiokande (Hyper-K)** is a world-leading neutrino experiment, building on success of Super-Kamiokande & T2K.

**Broad & ambitious physics programme** covering many neutrino sources as well as proton decay measurements.

**Water Cherenkov (WC) detector technology** provides huge target mass with excellent particle ID and reconstruction capabilities.



**Solar** 

**Atmospheric v** Supernova *v* 

## **Hyper-K's Water Cherenkov Detectors**

#### **Hyper-K Far Detector**



#### **Intermediate Water Cherenkov Detector**

- Measures  $\nu$  flux and cross-section of beam at ~1 km from source
- Moves vertically in  $~50$  m tall pit
	- $\circ$  spans off-axis angles of  $\nu$  beam for different  $\nu$  energy spectra
- $\bullet$  6 m tall x 8 m diameter tank with ~500 multi-PMT modules (mPMTs)

○ 8 cm PMTs:

- Better position resolution
- 1 ns timing resolution
- Additional directionality information
- mPMTs will also be used for WCTE
- Also being produced for portion of far detector photo-coverage

#### **Upgraded detector technologies need improved data analysis techniques**





## **Reconstruction in Water Cherenkov Detectors**

**Classification:** Particle type identification (PID)

Particles produce different types of rings due to interactions in water



**Regression:** Reconstructing particles' properties

- Location and time of PMT hits allow triangulating particle's position and direction
- Amount of charge observed at PMTs gives estimate of particle's energy

## **Machine Learning Reconstruction for WC**

Reaching limit of traditional maximum-likelihood reconstruction methods (**fiTQun**)

- Improved resolutions require more complex algorithms with fewer approximations
- Computation time is limiting factor: **1M events in fiTQun = 10,000s CPU-hours**
- Machine Learning (ML) and deep neural networks have potential to push reconstruction further
	- Potential to use all information without detector model approximations
	- Very fast once network is trained: **1M events with CNN < 100 CPU-hours or < 1 GPU-hour**



#### **Networks on 2D image-like data**

## **Image-like data for IWCD with mPMTs**

#### **19 PMT hit charges + 19 PMT hit times**





#### **Full cylinder is unwrapped onto flat image**

- One pixel per multi-PMT
	- 41 channels per pixel:
		- 19 charge (at each of the 19 PMTs per mPMT)
		- 19 time (first hit time of each PMT is digitized)
		- $\circ$  (x, y, z) positional encoding of mPMT location helps network learn geometric information
	- Tried other topological mappings with less success

## **Data Transformations and Augmentation**



Double cover transform for all events helps generalisation



Rearranging and duplicating the geometrical surface has several advantages

- Less dependence on choice of slice along barrel to unwrap cylinder
- All segments appear exactly twice, with minimal blank space
- **Circular boundary conditions** in both directions

Applying random transformations using detector symmetry effectively increases dataset



#### **ResNet event reconstruction for IWCD with mPMTs**



#### **Convolutional Neural Network based on ResNet-50**

- Initial 7x7 convolution with downsampling replaced by convolution over mPMT features
- Circular padding applied on each convolution to exploit cyclic boundary conditions

**Simulated for IWCD 3M each of**  $e, \mu, \pi^0, \gamma$  **(with**  $\gamma$  **to**  $e^+e^-$  **pair conversion at initial position)** 

- Uniform random position, isotropic directions, uniform energy 0 to 1 GeV above Cherenkov threshold
- 1.5M of each particle for training, 0.3M for validation, 1.2M for final evaluation

**Trained separate models for each task** for ~ 12 hours on 4 x A100 GPUs

- Single 4-class network for PID classification of  $e, \mu, \pi^0, \gamma$
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## **Regression results**

#### **Basic cuts:** > 25 hits & fully contained event

#### **Reconstruction resolutions all reduced by 40 - 70%**



## **GRANT: Graph Network for Hyper-K Far Detector**



#### **Features at each node (hit PMT)**

- **PMT** hit charge
- **PMT** hit time
- **PMT** location

#### **Nearest neighbour graph**

- Physical proximity of PMTs
- or charge, time proximity
- or both

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#### **ResGatedGraphConv**

- Graph convolution: aggregates information from neighbouring nodes
- Gate mechanism: adaptively controls amount of information passed between nodes
- Residual connection: Adds original node information to updated information for enhanced gradient propagation

Pooling layer followed by fully connected network provides 1D array of output features (PID variables, reconstructed quantities)

## **GRANT GNN Results**





**fiTQun** 7.0% resolution, 0% bias 6.0% resolution, 0% bias

Traditional method (fiTQun) tuned to MC to avoid / correct for bias, need to investigate bias source in GRANT

Vertex position reconstruction is not performing well in GRANT, under further investigation

**CERN T9 beam 0.2 to 1.2 GeV**

**WCTE**

**Unique opportunity to study**  $\tt{tagged\ e^{\pm},\ \mu^{\pm},\ \pi^{\pm},\ p^{\pm}\ \text{and}\ \gamma\ \text{beam\ of}}$ **known momentum, position, direction**

**Trigger**

**Hole** 

Permanent **Halbach Magnet**

- First beam run scheduled Oct-Nov 2024
- **Physics measurements include Cherenkov** emission and leptonic & hadronic scattering

**Trigger**

**Hole Counter**



Main purpose is to develop new hardware, techniques and measurements to reduce interaction physics and detector systematic uncertainties in future  $\nu$  experiments

**Aerogel cherenkov (particle ID)**

**charged particle configuration**

**tagged photon configuration**

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**Hole Counter** 

 $e^{\frac{1}{2}}$ 

**Hodoscope**

- ResNet and GRANT both adapted to WCTE Detector geometry with ResNet currently showing comparable performance to IWCD on simulated MC samples
- Potential to demonstrate and validate ML-based reconstruction for WC detectors on real data in real-world experimental conditions

## **Summary**

Hyper-Kamiokande, the next-generation water Cherenkov neutrino detector experiment has begun construction to start operation in 2027

• Both the far detector and IWCD will require new techniques to improve reconstruction, suppress backgrounds and reduce systematics

Machine learning can avoid the likelihood model approximations of traditional methods

- CNN and GNN architectures already outperforming traditional methods
	- 40 70% improvement in IWCD position, direction and energy resolutions
	- $\circ$  New analyses made possible from new  $e / \gamma$  discrimination capability
- Additional benefit of huge increase in speed of reconstruction

WCTE provides unique opportunity to demonstrate ML methods with real-world data

• First data taking with beam scheduled Oct - Nov this year

### **Appendix**

### **ResNet event reconstruction for IWCD**

#### **Trained models on simulated IWCD data**

- Generated 3M each of e,  $\mu$ ,  $\pi^0$ ,  $\gamma$  (with conversion  $\gamma$  to  $e^+e^-$  pair at initial position)
	- Uniform random initial position in entire detector, isotropic random initial directions
	- Uniform random energy 0 to 1 GeV above Cherenkov threshold for given particle type
- Split into training, validation and test sets
	- Training: 1.5M of each particle for training
	- Validation: 0.3M of each particle to monitor training and to choose the best trained model
	- Testing: 1.2M of each particle; enough stats to compare small differences between models e.g. differences in e vs mu performance around 99.9% accuracy
- Trained each model for  $\sim$  12 hours on 4 x A100 GPUs

#### **Classification**

- Single 4-class network for PID classification of e,  $\mu$ ,  $\pi^0$ ,  $\gamma$
- Cross-entropy loss, batch size=1024, Adam optimiser, learning rate=0.002

#### **Regression**

- Six separate networks for position, direction and energy of  $e$  and  $\mu$
- Huber loss with delta=0.1, batch size=1024, Adam optimiser, learning rate=0.002

## **Direction reconstruction**



#### **Momentum reconstruction resolution**





## **3D position reconstruction**



#### **Muon position reconstruction (longitudinal & transverse)**



#### **Electron position reconstruction (longitudinal & transverse)**



## **IWCD Regression summary**

- Position, direction and energy for both muons and electrons
- Separate training run for each particle / quantity
- Trained for 12 hours in each configuration # epochs varied by training set size
	- Trained each model on one Narval GPU node (4 x A100 40 GB GPUs) for 12 hours
	- Electron dataset is much larger (from large e/gamma separation dataset)
	- FC cuts also reduce dataset size
	- Could maybe benefit from larger muon dataset to match electrons



- For comparison, "ResNet old" refers to results with:
	- No double cover, no augmentations, no hit timing information, no feature scaling
	- Polar and azimuth angles for direction reconstruction
	- 20 epochs for all cases

## **IWCD Regression summary**



Resolutions defined as 68th percentile of 3D distance between true and reco positions, angle between true and reco directions, residual of |reco - true| energy, etc.

Biases defined as mean of (reco - true) values

## **ResNet for pile-up identification in IWCD**

#### **Study of single-vertex vs multi-vertex classification**

- **IWCD will see multi-vertex** pile-up events due to close proximity to neutrino beam
- Trained network to classify multi-track events as single or multiple vertices
- Trained on particle gun events with 2+ particles from a single vertex or from two vertices
- Tested on samples using realistic neutrino interactions generated by GENIE or NEUT

#### **Single-vertex multi-track event Pile-up event**





## **Pile-up training and testing samples**

For all events:

Each vertex is a random uniform position in the tank, random initial time from Gaussian with width of 25ns

For training:

- 2.5M events each for single or multi-vertex
	- For single-vertex all particles start at the same vertex (position and time)
	- For multi-vertex particles randomly split between two vertices
- 2 to 5 particles simulated per event, with 'unbiased' distributions to avoid model bias
	- Each particle randomly chosen from electron, muon, neutral and charged pions
	- Each particle has random isotropic direction
	- Total energy of all particles uniformly distributed from 0 to 2 GeV

For testing:

- Number, type, energies, direction of particles determined by neutrino interaction MC
- $\bullet$  ~1M events produced using each of NEUT and GENIE
	- For single-vertex take a single neutrino interaction
	- For multi-vertex take two neutrino interactions

#### **Pile-up results**

#### **Single vertex acceptance vs multi-vertex rejection**



Working nicely with NEUT/GENIE MC events after training with particle gun MC

#### **Pile-up results**



vertices close to each other in space

## with small towall distance

#### **Pile-up results**



Some degradation of performance at lower energies



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## **Problem with WCTE in ResNet for regression**

- **Problem:** 16 columns + circular boundaries + CNN translation invariance = identical network output after 180° rotation of detector about its axis
	- Network learns locations on tank from pattern of filled/unfilled pixels
	- But translations equivalent to 180° tank rotation have same pattern so network output is identical for a 180° rotated event
	- Need to break symmetry for network to learn position and directon
- ResNet performs 3x3 convolutions and maxpools with a stride of 2
	- Considering the downsampling, the translation invariance is only unbroken for translations by number of pixels equal to powers of 2
- WCTE has 16 columns
	- Horizontal 180° rotation of the tank about its axis in 3D is the same as translating the 2D double-cover image by 8 pixels
	- So the network cannot distinguish between any event and the equivalent with the tank rotated by 180°
	- Vertical 180° rotation is equivalent to 9 pixel translation so the invariance is broken due to the stride of 2
- IWCD has 40 columns so didn't see this problem
	- After 2 downsamples, the a 20-pixel translation for 180° tank rotation becomes a 5-pixel translation
	- With stride of 2, there is translation invariance of only even number of pixels
	- So it can learn the difference between an event and the equivalent event rotated by 180°



## **Problem with WCTE in ResNet for regression**

- **Problem:** 16 columns + circular boundaries + CNN translation invariance = identical network output after 180° rotation of detector about its axis
- Solve problem with Positional encoding: provide geometrical information as extra channels
	- Each mPMT pixel now has 41 channels of data instead of 38
		- $\blacksquare$  19 charge channels + 19 time channels = 38
		- $\blacksquare$  + 3 channels for x, y, z position of the middle of the mPMT
	- Also added option to provide channels for mPMT orientation
- Adding the mPMT position channels allowed it to successfully learn particle position and direction
	- Takes longer to converge, but once it does the performance is improved
	- No benefit seemed to come from also adding orientation, only position seemed to help
	- Also tried one-hot encoding channels of mPMT locations for network to learn 3D geometry
		- Same eventual performance within statistical errors, but slower to train



● The **charged particle configuration** includes **Aerogel Cherenkov counters** with different refractive indices chosen for each beam momentum, for tagging of electrons and muons through their Cherenkov threshold; **Time of Flight** (TOF) detectors with 100 ps timing resolution provide identification of the heavier hadrons ( $p, \pi, K$ , etc.)



- A **hodoscope** measures the deflected positron's energy to determine the photon's energy
- July 2023 beam test successfully demonstrated capability of both beam monitor configurations
- Data taking is scheduled for 6 weeks Oct-Nov 2024 with additional beamtime expected in 2025

### **WCTE Muon momentum reconstruction**

- Trained on true fully contained events with  $> 10$  hits
- Test on fully contained events with  $> 25$  hits and towall  $> 1$  m



### **WCTE Electron momentum reconstruction**

- Trained on true fully contained events with  $> 10$  hits
- Test on fully contained events with  $> 25$  hits and towall  $> 1$  m



### **WCTE Momentum bias against to wall distance**



## **WCTE Electron / muon PID**





99.9% muon rejection

fiTQun performs poorly without additional cuts on towall, dwall, etc.

## **WCTE Reconstruction summary**



WCTE ResNet performance almost as good as IWCD ResNet and better than IWCD fiTQun Direction resolution most significantly reduced compared to IWCD, probably due to lower granularity of PMTs to resolve particle direction

#### **GRANT: Machine Learning based algorithm for reconstruction**



## **Events at high energy**

- o Large number of PMTs triggered (around **3000 hit PMTs for e- event at 500 MeV).**
- o For each PMT, **5 distinct pieces of data** are collected: Position (x, y, z), Charge, Time
- **Result: MASSIVE DATASET**
- events exhibit a distinctive  $\circ$  These geometrical shape (like a ring). Our goal is to identify patterns using the 5 pieces of information from each hit PMT.
- Graphs are an excellent tool for this  $\circ$ purpose!

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#### **GRANT: Machine Learning based algorithm for reconstruction**



#### **Main Features**

# **ResGatedGraphConv.**

- **Graph Convolution: Aggregates information from** neighboring nodes to update each node. (graphbased learning)
- **Gate Mechanism: Uses a weight (between 0 and 1) to** control the amount of information that is passed from one node to another. (adaptive control of information flow)
- **Residual Connection: Adds the original node** information to its updated information, facilitating gradient propagation. (enhanced gradient propagation)
- It's a neural network  $\bullet$ layer designed to work with data structured as graphs.
- It combines  $\bullet$ elements of graph convolution, gating mechanisms, and residual connections.















For events close to the wall: GNN > Existing software  $\Rightarrow$  potentially increase FV

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#### Performance comparation: GRANT vs existing software

a) e/mu

b) e/pi0 c) e/gamma d) Energy

e) Vertex



### **Traditional reconstruction method**

fiTQun: Likelihood-based reconstruction for higher energies

- Originally developed for Super-K detector ○ Based on algorithm of MiniBooNE: <https://arxiv.org/abs/0902.2222>
- Uses full information of unhit PMTs  $+$  time & charge of hit PMTs:



- Probabilities calculated based on direct  $+$  scattered  $+$  reflected light
- Likelihood ratios used to distinguish particle types and single-ring / multi-ring event topology hypotheses

## **Topological map to square**

Alternative map onto square with boundary conditions preserving topology of cylinder

- Cut open along barrel to centre of end caps (solid line)
- Deform onto square, keeping density of PMTs constant
- **Place mPMTs onto nearest pixel**
- Use boundary conditions identifying edges of square (indicated by arrows)
	- Pad image with copy of pixels from the corresponding edge

$$
X_{\pm} = W(\rho, z) \frac{\pi \pm \phi}{2\pi}
$$
  

$$
W(\rho, z) = \sqrt{\frac{\rho^2 + 2Rz + RH}{R^2 + RH}}
$$
  
  
Soive differential eq. for  
constant 3acobian  

$$
dX_{+} dX_{-} = \left| \frac{\partial(X_{+}, X_{-})}{\partial(\rho, \phi)} \right| d\rho d\phi
$$









## **Segmentation networks**

- Classification networks can be extended to perform segmentation
	- Deconvolutions and upsampling reverse convolutions and downsampling
	- Provides output value for each pixel
	- Currently using U-Net and FRRN
- $\bullet$  Starting development with  $\pi^0$  events
	- *π 0* decay to produce two *γ* rings
	- $\circ$  Higher energy  $\pi^0$  have overlapping rings





