Machine Learning Methods for Track Classification in the AT-TPC

M.P. Kuchera\textsuperscript{a}, R. Ramanujan\textsuperscript{b}, J. Z. Taylor\textsuperscript{a}, R. R. Strauss\textsuperscript{b}, D. Bazin\textsuperscript{c}, J. Bradt\textsuperscript{c}, Ruiming Chen\textsuperscript{a}

\textsuperscript{a}Department of Physics, Davidson College, Davidson, NC 28035, USA
\textsuperscript{b}Department of Mathematics and Computer Science, Davidson College, Davidson, NC 28035, USA
\textsuperscript{c}National Superconducting Cyclotron Laboratory, Michigan State University, Lansing, Michigan, 48824, USA

Abstract

We evaluate machine learning methods for event classification in the Active-Target Time Projection Chamber detector at the National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University. An automated method to single out the desired reaction product would result in more accurate physics results as well as a faster analysis process. Binary and multi-class classification methods were tested on data produced by the $^{46}$Ar(p,p) experiment run at the NSCL in September 2015. We found a Convolutional Neural Network to be the most successful classifier of proton scattering events for transfer learning. Results from this investigation and recommendations for event classification in future experiments are presented.

Keywords: machine learning, neural networks, classification, active targets, time projection chamber

1. Introduction

1.1. Challenges of data analysis in time projection chambers

A time projection chamber (TPC) is a gas-filled chamber used for detecting charged particles. An electric field is formed in a TPC between a cathode and anode on either end of the detector. As a charged particle travels through the gas, it ionizes the atoms of the gas, leaving electrons that drift in the electric field in the direction of the anode in the detector chamber. By measuring the location and time of arrival of these electrons on the anode,
the particle’s three-dimensional track can be reconstructed with nearly $4\pi$ angular coverage. Since this type of detector records every type of event, selecting the events of interest is a challenge in TPC experiments.

1.2. Classification in the AT-TPC

The Active-Target Time Projection Chamber (AT-TPC) is a detector where the nuclei in the gas inside the chamber also act as the target for nuclear reactions. This detector is used for low energy nuclear physics experiments with radioactive nuclei at the National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University [1]. An active target provides advantages over a solid target by allowing reactions to be measured over a wide range of energies. The incident beam loses energy as it travels through the gas, and reactions can occur anywhere within the gas volume. This allows excitation functions to be measured using a single beam energy.

Events of interest are assumed to be those that have small errors in the track-fitting stage of the analysis, which is currently performed using a naïve Monte Carlo method. The procedure is to fit the trajectory of the reaction products as if they were the product of interest, and then to conclude otherwise if the Monte-Carlo fitting results in a high error. A more informed method would first determine the particle type and move forward in the analysis only with the data of interest. We propose to use supervised machine learning to classify events in the detector on the basis of the spatial data and charge deposited on each pad by the reaction product. This allows for event classification early in the analysis process. Proceeding in the analysis with only events of interest allows for the improvement and fine-tuning of analysis methods, since these do not have to handle unexpected event types appropriately. In addition, this would reduce the error attributed to contaminated data in the analysis process.

This work used data from the $^{46}\text{Ar}(p,p)$ experiment that ran in September 2015 [2]. For this experiment, the AT-TPC was connected to the ReA3 beam line. The pad plane end of the detector was tilted to an angle of $6.2^\circ$ with respect to the magnetic field. The detector’s active volume was filled with isobutane gas at a pressure of 19.2 torr and placed in a 1.68 T magnetic field created by a solenoid magnet surrounding the detector [2]. An electric field of approximately 9.5 kV/m was induced in the active volume.
The signal from each pad in the pad plane was sampled at 512 time buckets per event and the clocking frequency of the electronics was set to 12.5 MHz. Ionized electrons were amplified by the application of a $-450$ V potential to the Micromegas mesh with respect to ground [2].

The $^{46}$Ar experiment ran for 12 days and produced approximately 12 TB of raw data. After initial cuts on the data to remove events from beam contaminants, we estimate that approximately 10% of the remaining data comprises proton elastic scattering events, which is the reaction of interest to the researchers. This value was calculated from manually labeling a small subset of the raw data, which is discussed in Sec. 4.1. Our goal for this work was to create a model to automatically select these proton scattering events from the spatial and charge information for each event.

2. Machine Learning Background

The current approach for identifying events of interest from the experimental data relies on Monte-Carlo optimization techniques in conjunction with a $\chi^2$-based goodness-of-fit test. In this work, we propose using machine learning methods instead for the problem of track classification in the AT-TPC. We start with a dataset comprising descriptions of events recorded in the detector. Each event is represented as a vector of real numbers (of fixed length) and is termed an example. Each component of this vector is called a feature. Attached to every example is a label, indicating the identity of the particle that generated the said track — for example, proton or non-proton. The learning task is to find a surface $h$ (dubbed a separating hyperplane) that partitions the data such that all tracks corresponding to proton events lie on one side of $h$, while all non-proton events fall on the other side. Formally, we seek a function $h_\theta : \mathbb{R}^n \mapsto \{0, 1\}$, parameterized by a set of weights $\{\theta_1, \theta_2, \ldots, \theta_n\}$, that minimizes a cost function $J(\theta)$. The function $J$ is a cumulative measure of the classification errors made by the decision surface $h_\theta$. Fig. [4] provides the visual intuition behind this task, using a simplified scenario where every event is represented by a two-dimensional point and a line is an adequate decision boundary. In practice, however, the events are usually not easily separable; thus, we also investigate the effectiveness of non-linear separating surfaces for the track classification problem. Appropriate values of the weight parameters $\theta$ are found using standard optimization

3
techniques like gradient descent. After preliminary explorations, we focused our study on three model families, which are described below.

Figure 1: A separating hyperplane for a classification problem where each example is represented by two features $f_1$ and $f_2$. While the two classes are cleanly separated by a line in this example, more complicated data distributions may require the use of non-linear surfaces.

2.1. Logistic regression

Logistic regression is a classic approach in statistics and machine learning for modeling the probable value of a binary variable $y$. If we (arbitrarily) assign proton tracks the label $y = 1$ and non-proton tracks the label $y = 0$, then given an example $x \in \mathbb{R}^n$ representing an event, the logistic regression model calculates the probability that this was a proton event as:

$$Pr(y = 1|x) = h_\theta(x) = \frac{1}{1 + e^{-\theta^T \cdot x}}$$

The expression $\theta^T \cdot x$ represents a weighted linear combination of the input features. This operation is composed with a mean function — in this case, the logistic function $\sigma(z) = 1/(1 + e^{-z})$ — to ensure that the output of the model remains bounded by $[0, 1]$. The parameters $\theta$ are fitted by minimizing the binary cross-entropy loss function:

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} (y_i \log \hat{y}_i + (1 - y_i) \log (1 - \hat{y}_i))$$

(1)
where $m$ denotes the number of examples in the dataset and $\hat{y}_i = h_\theta(x_i)$ is the model’s prediction for the $i^{th}$ event $x_i$. Smaller values of this loss function $J$ are achieved when the model’s predictions $\hat{y}$ more closely match the true labels $y$. While the treatment above considers the scenario of binary classification, where each example belongs to one of two categories, logistic regression can be extended in a straightforward fashion to the multi-class setting as well — we refer the reader to [3] for further details.

2.2. Neural networks

The term neural network describes a large class of models that are loosely inspired by the processes that drive learning in biological neurons. They have been successfully applied to problems from a number of challenging domains, including image recognition [4], autonomous driving [5], game-playing [6], as well as in experimental physics [7]. A neural network comprises a collection of units (“neurons”) that form a graph. Each unit accepts inputs from other units, aggregates them in some non-linear manner and produces an output that may be consumed by other units. This composition of neuronal units means that such networks are able to learn very complex decision surfaces; indeed, under some mild assumptions, it can be shown that neural networks with a finite number of units can approximate any continuous function to arbitrary precision [8]. While neural networks are highly configurable, only certain network architectures and neuronal unit choices find wide use in practice. In the next two subsections, we describe the two neural network models that were explored in this work.

2.2.1. Fully-connected feed-forward neural networks

In this classic neural network architecture, every node computes a linearly weighted sum of its inputs (plus a bias term). A non-linear activation function is then applied to this sum to produce the unit’s output. We use the rectified linear function ($f(z) = \max(0, z)$) in this work, as it produced superior results to other common choices like the hyperbolic tangent and logistic functions. The left panel in Fig. 2 visually depicts the computation performed by each artificial neuron.

In a fully-connected architecture, the individual neurons are organized in a layered fashion as depicted in the right panel of Fig. 2. Every unit in a given layer $i$ accepts inputs from every neuron in layer $i - 1$ and each connection is associated with its own weight. The term feed-forward refers to the fact that
Figure 2: Left: A single neuronal unit. The function $f$ is a non-linear activation function. Right: A fully-connected feed-forward neural network formed by connecting together several artificial neurons.

the network is acyclic: information flows from the features $x$ that comprise the input layer, through one or more hidden layers of neurons, to produce a result at the output layer, with no feedback loops. Networks with more than one hidden layer are called deep networks, and the term deep learning refers to the set of techniques used to train such networks [9]. The overall output of the model $\hat{y} = h_\theta(x)$ is a composition of applications of the activation function to the input features $x_i$ and is the estimated probability that the input example corresponds to a proton event $Pr(y=1|x)$. As with logistic regression, the parameters of the model (i.e., the weights attached to each edge in the network) are fitted by minimizing the cross-entropy loss defined by Eq. 1 using optimization techniques like gradient descent. The backpropagation algorithm offers a method for efficiently computing the gradient of the loss function with respect to the network weights by caching the results of intermediate derivatives and avoiding their repeated recomputation [10].

2.2.2. Convolutional neural networks

A convolutional neural network (CNN) is a learning model that is particularly suited for applications that operate on grid-like data, such as time series (a 1-dimensional grid of samples) or images (a 2-dimensional grid of
While their early success in problems like recognizing hand-written zip codes \cite{11} hinted at their potential, CNNs truly came into their own in 2012 when the \textit{AlexNet} model resoundingly won the ImageNet visual recognition contest \cite{12}. CNNs have since completely revolutionized the field of computer vision, and are central to state-of-the-art methods for many challenging problems such as object recognition \cite{4}, image segmentation \cite{13}, and image captioning \cite{14}. More pertinently, CNNs have also proven to be effective at certain tasks in high-energy physics — for example, Aurisano et al. successfully used CNNs to recognize neutrino events in the NOvA experiment at Fermilab \cite{15}, albeit on simulated data. In this work, we study the efficacy of CNNs in the AT-TPC track classification domain by framing the problem as a visual recognition task. We train the network to make predictions based on plots of two-dimensional projections of events recorded in the detector.

We now provide a sketch of the main ideas underlying CNNs and refer the reader to \cite{9} for a more comprehensive treatment. A CNN model is built by arranging three kinds of layers, described below, in various configurations.

\textbf{Convolutional layer} CNNs use the discrete convolution operation to identify distinctive visual characteristics in an image, like corners, lines and shapes. This is a linear transformation that maps a 3-dimensional input volume to a 3-dimensional output volume. Formally, consider an input volume (for example, an image) $I$ of dimensions $h \times w \times c$, where $h$ represents the height of the volume, $w$ represents the width, and $c$ the number of channels (for RGB images, $c = 3$). An $m \times n \times s$ convolutional layer $F$ comprises a stack of $s$ 2D convolution kernels (also called filters), each of which has height $m$ and width $n$. Each filter also extends fully through the channel dimension $c$, and the values produced by the channel-wise convolutions are simply summed up along this axis. The result of convolving $F$ by $I$ is given by:

$$
(F * I)(i, j, k) = \sum_{p=0}^{m-1} \sum_{q=0}^{n-1} \sum_{r=1}^{c} I(i + p, j + q, r) \cdot F(p, q, r, k)
$$

where $(F * I)(i, j, k)$ refers to the value at position $(i, j)$ in the $k^{th}$ channel of the output volume. Fig. 3 presents this operation visually. Typically, the spatial extent of each kernel is much smaller than the dimensions of the input volume, so that $m \ll h$ and $n \ll w$. Thus,
Figure 3: The first step in the convolution of a $5 \times 5 \times 3$ image by a single $3 \times 3$ filter. For each channel of the input, we compute a sum of the highlighted pixel values weighted by the corresponding values in the convolution kernel. The channel-wise results are then summed up to produce the indicated entry in the output feature map. The remaining values of the feature map are populated by sliding the kernel over the input and repeating the operation. A convolutional layer comprises many such filters, each of which produces its own feature map. The weights of the kernels are determined by the learning process.

Each kernel is highly localized in its sensitivity, and models the notion of a receptive field that is a feature of the mammalian visual cortex [16]. The borders of the input volume are usually padded with an appropriate number of zeros to ensure that the output volume has the same width and height as the input. The output thus has dimensions $h \times w \times s$, and each slice of this volume along the $s$ dimension is referred to as a feature map.

**Activation layer** An activation layer typically operates on the output of a convolutional layer and applies a non-linear function to its input in an element-wise fashion. The rectified linear unit (ReLU), defined as $f(x) = \max(0, x)$, is a commonly used activation function that permits
effective learning in deep CNNs [12,17].

**Pooling layer** A convolutional layer produces a number of feature maps, each of which have the same height and width as the input volume. When a CNN contains many such layers, the memory and computational requirements of the model grow very quickly. Pooling layers alleviate this problem by downsampling the input volume along the spatial dimensions. A commonly used pooling operator is max pooling, which replaces the values in an $m \times n$ region of the input with a single value corresponding to the maximum of those values [18]. The degree of overlap between the pooled regions can be adjusted to reduce the loss of information. Pooling also makes the performance of the network robust to small translations of the input [9].

In addition to the specialized layers described above, a typical CNN also utilizes a fully-connected topology (as seen in Sec. 2.2.1) in the last one or two layers preceding the output layer. The role of these dense layers is to combine the features extracted by the prior layers to produce a categorical prediction. A schematic diagram of the overall architecture is shown in Fig. 4. As before, the network is trained by minimizing the cross-entropy loss function given by Eq. 1. The learning process tunes the weights associated with the fully connected units, as well as the weights of the convolution kernels.

![Figure 4: The stages comprising a typical CNN model. In the first stage, the pixel-level data from the input is passed through multiple convolution, activation and pooling layers to extract high-level features describing the image. These features are then used by the latter stage to classify the example.](image)
High-performing CNN models are typically composed of many layers. For example, the VGG16 model that won the ImageNet visual recognition challenge in 2014 uses 16 weight layers — 13 convolutional layers (combined with ReLU activations) and 3 fully-connected layers, with max-pooling layers inserted at various stages [19]. The model has $\sim 138$ million parameters.

Training such a network from scratch, with random initialization, requires extremely large labeled datasets (ImageNet has $\sim 14$ million examples [20]) and takes days on high-performance GPUs. For applications with limited training data, an alternative is to use a pre-trained network [21] (like VGG16 trained on ImageNet) in one of two ways:

- As a preprocessor: One could remove the final fully-connected and output layers from the pre-trained model and process each training image (for example, two-dimensional plots of AT-TPC events) by passing it through the network. This produces a fixed-length vector representation of the original image, that can be then be used as the input to a simple classification algorithm, like logistic regression.

- As a weight initializer: One could use the weight settings of the pre-trained model as a starting point, and fine-tune these using gradient descent approaches to improve the model’s performance on the new dataset. A very small learning rate is used to ensure that the original weights are not subject to excessive distortions.

We explore both these approaches in this work.

3. Model Fitting Methodology

There are a number of practical considerations when one builds machine learning models for a particular application. Learning algorithms often have a number of hyperparameters — free variables whose values must be fixed prior to commencing the model fitting process — whose settings can have a large impact on the performance of the model. These hyperparameters must thus be chosen thoughtfully. Further, care must be taken when measuring the performance of the model, to ensure that the reported results are unbiased and not overly optimistic. This section provides an overview of our model fitting methodology.
3.1. Combating Overfitting

In statistics, the term overfitting refers to the situation where a model captures the regularities in the training dataset so well that it fails to generalize effectively to unseen examples [3]. This problem is particularly acute when a model has high capacity (i.e., the ability to represent complex decision boundaries) or has a large number of parameters relative to the size of the training data. Fig. 5 provides a visual illustration of overfitting. In the remainder of this section, we describe some techniques that were used to address overfitting in our work.

Figure 5: The above are scatter plots of an artificial dataset with two features \(f_1\) and \(f_2\). This is a binary classification task, with red and blue corresponding to the two class labels. The circles are points used for training the model; the triangles are additional data points that are not used for training purposes but to evaluate the learned model’s ability to generalize. The shaded regions and their boundaries represent the fitted decision surface. In the left panel, we have a linear model that is well-fit: while it misclassifies some of the training data, it also makes few errors on the unseen data points. The right panel depicts an overfit model, i.e., one that correctly classifies every training example, but makes many mistakes on new, unseen examples.

3.1.1. Train-Test-Validation Splits

One common method for estimating the generalization error of a learned model is to evaluate its performance on a set of held out data, that was
not used during the training process. The original collection of examples is divided into a training, a validation and a test set. The data in the training set is used for the fitting process. The validation set is used to compare different hyperparameter settings (for example, the size and number of hidden units in a neural network) and choose the best performing configuration. The test set is used to report the performance of the final model, and offers an unbiased measure of the model’s quality. We follow this protocol in this work: all model performance figures in Sec. 4.4 are reported on a held out test set.

3.1.2. Early Stopping

For models that are fitted using an iterative procedure — for example, neural networks trained with stochastic gradient descent — one can mitigate the effects of overfitting by monitoring the progress of the learning process. In particular, one can plot a learning curve like that shown in Fig. 6 that tracks the value of the model’s loss on the training and validation sets over time. The fitting process can then be stopped at the point where the two losses start diverging, which signals the onset of overfitting.

![Learning Curve](image)

Figure 6: A learning curve depicting the value of the model’s loss on examples in the training set (blue) and the validation set (red) over time. The x-axis indicates epochs of training, where one epoch represents one complete pass through the dataset for stochastic gradient descent. The early stopping point in this example occurs at epoch 10, indicated by the vertical black line.
3.1.3. Regularization

Regularization is a mathematical technique that discourages the fitting of overly complex models by including a penalty term in the loss function being minimized by the training process [3]. The squared L2 norm of the model’s parameter vector $\theta$ is a common choice for the regularizer; when combined with Eq. 1, it yields the following modified binary cross-entropy loss function:

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} (y_i \log \hat{y}_i + (1 - y_i) \log (1 - \hat{y}_i)) + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$$

Here, $\lambda \geq 0$ is a hyperparameter that controls the strength of the regularization. Larger values of $\lambda$ cause the weights in the model to shrink and yield simpler decision boundaries [3]. The ideal setting of $\lambda$ for a given problem can be found by sweeping a range of values and evaluating the performance of each resulting model on the validation set.

3.1.4. Dropout

Dropout is a regularization technique that is widely used when training deep neural networks [22]. At training time, before each batch of examples is presented to the network, a random subset of the neuronal units in the model (along with their connections) is temporarily removed. The parameters of the resulting pruned model are adjusted as per the usual training procedure. A different thinned model is then sampled before the next batch of examples, and this process is repeated until the end of the training phase. At test time, the trained connection weights in the model are scaled by the dropout probability $p$, which is a hyperparameter. This randomized dropping of units during training prevents complex co-adaptation among neurons, where a certain unit’s usefulness becomes closely coupled to the outputs of several other specific units [22]. Minimizing such co-adaptation is an effective way to combat overfitting and dropout is thus used by several well-known deep models such as AlexNet [12] and VGG16 [19].

3.2. Performance Metrics

In this work, we measure the performance of our machine learning models using three metrics that are widely used by the information retrieval and machine learning communities: precision, recall, and F1 score [23]. Compared to more intuitive measures like classification accuracy, these metrics are more
effective at conveying the nuances of a model’s performance and provide insight into the nature of its errors. In the AT-TPC track classification domain, we are particularly interested in a model’s ability to correctly identify proton events, and these metrics enable us to characterize this precisely.

| True Class | Predicted Class | # protons correctly classified | # non-protons correctly classified |
|------------|----------------|--------------------------------|----------------------------------|
| Positive   | Proton         | No                             | No                               |
| Negative   | Non-Proton     | No                             | No                               |

Figure 7: The elements of a confusion matrix for a binary classification problem. Each row represents the class predicted by the classifier, while each column represents the true class label. The left matrix presents the terms used to describe each entry. The right matrix interprets these terms when applied to AT-TPC data. A perfect classifier induces a left diagonal confusion matrix.

The definitions of precision and recall are best understood by first examining a structure known as a confusion matrix. A confusion matrix tabulates the predictions made by a binary classifier and places them in one of four cells, as shown in Fig. 7. This figure also presents the terms used to refer to the entries in a confusion matrix and a contextual example using AT-TPC data categories. Precision is a measure of a classifier’s soundness — in the AT-TPC context, it quantifies how often a model is correct when a track is identified as having been generated by a proton. Using the terminology of Fig. 7, we can define precision formally as follows:

\[
\text{precision} = \frac{TP}{TP + FP}
\]

Recall, on the other hand, is a measure of a classifier’s completeness — it measures how many proton events were successfully picked out by the model.
from the set of all true proton events. Formally, the recall is defined as:

$$\text{recall} = \frac{TP}{TP + FN}$$

In most applications, higher precision often comes at the cost of lower recall, and vice versa. Thus, these two metrics are usually measured and reported together. Alternately, their harmonic mean is reported as a single value known as the F1 score:

$$F1 = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

All three metrics are bounded by $[0, 1]$, with a higher value indicating better performance on that measure. The results presented in Sec. 4.4 report the precision, recall and F1 score of the proton class.

4. Applications to $^{46}\text{Ar}(p, p)$

To test our methods, we attempt to classify protons against all other reaction products and other charged particles detected in the AT-TPC during the $^{46}\text{Ar}(p, p)$ experiment (e13306b) at the NSCL. Ideally, the desired reaction product will be classified early in the analysis workflow. This would occur either in real-time as the experiment runs, or shortly after, on minimally processed data. Realizing this goal requires access to a trained classifier before the experimental data becomes available. One way to achieve this is to fit a model using simulated data instead. This is an example of transfer learning, where the algorithm is trained using a different dataset than the actual data we are interested in classifying. To investigate the feasibility of this goal, we focus on three machine learning tasks:

- training and testing with simulated data,
- training and testing on real experimental data, and
- transfer learning.

While testing our performance on simulated data does not achieve our goal of classifying experimental data, this setting provides us with an upper-bound
on the performance that can be achieved by our models.

In each of the above settings, we also consider two different framings of the learning task: as a binary classification problem, where the model makes a determination of whether an event is a proton scattering event or not, and as a multi-class problem, where the model categorizes an event as one of “proton”, “carbon”, or “other”. The latter approach is motivated by the fact that carbon atoms are a very common by-product in the $^{46}Ar(p, p)$ experiment and the physics of their behavior in the detector is simulable. This allows us to generate synthetic datasets that more closely match the experimental data. We also investigate the question of whether having more fine-grained distinctions among events improves the performance of our models. The “other” label is a catch-all category that covers event types that we cannot simulate accurately — we resort to simple uniform random noise to mimic these events in our synthetic data.

4.1. Experimental training data

Experimental data was taken from the experiment described in Sec. 1.2. Supervised machine learning requires labeled data for both training and evaluating the performance of a model. Therefore, a sample of events from the $^{46}Ar(p, p)$ experiment was manually labeled for model building purposes. Tab. 1 summarizes the number of events in our hand-labeled experimental dataset. For the results presented in this paper, we randomly selected 2151 events to create the training set, with 15% of those events used for validation during training, and reserved the other 538 events for evaluating the model. The size of this dataset is limited only by human effort in labeling the data, as we have over $10^6$ events from the experiment [24].

| Event Type | Simulated | Experimental |
|------------|-----------|--------------|
| Proton     | 28000     | 663          |
| Carbon     | 28000     | 340          |
| Other      | 28000     | 1686         |
| **Total**  | 84000     | 2689         |

Table 1: Labeled dataset sizes
4.2. Simulated training data

By simulating data, we can create a labeled dataset of proton and carbon events of any desired size. We sample uniformly from $z$, $\phi$, and $\theta$, as opposed to a more realistic distribution, to have better representation of rarer events in our model. Additionally, we filter out all simulated tracks that do not contain at least 150 hits in the pad plane, and whose average distance from $(x, y) = (0, 0)$ in the $xy$-plane is less than $135\text{mm}$, to ensure that our simulated charged particle events resemble the ones we observe in our experimental data.

Using the experimental specifications of the $^{46}\text{Ar}(p, p)$ experiment described in Sec. 1.2, we simulate the ideal detector response to proton and carbon tracks in the detector volume using the `pytpc` software package [1]. This package uses the Bethe-Bloch and Lorentz force equations, which track the particle through the detector volume, and models electron diffusion to produce a pad plane projection with full charge trace information. The simulation produces data in the same format as the real experimental data. Tab. 1 presents the size of the simulated dataset used in this work. The algorithm is trained on 60,000 events randomly selected from the overall set, with 15% of those events used for validation during training. The models are then evaluated on the remaining 24,000 simulated events. For transfer learning tasks, the training set size was 60,000 events, with 15% again used for validation, and the full set of 2689 labeled experimental events was used for model evaluation.

In our simulated proton and carbon events, we have a version of the data where we add random noise points to each track in hopes that our dataset more closely resembles the noisy data recorded in the highly-efficient AT-TPC. We add a random number of points at random $(x, y, z)$ coordinates within the detector chamber, each with a random charge value. Both the point count and the charge per point were generated from their own respective distributions based on statistics collected from data from the $^{46}\text{Ar}(p, p)$ experiment. Fig. 8 presents examples of our simulated events, with and without the presence of random noise.

4.3. Detector volume discretization

Since our models require samples to be represented as fixed length feature vectors, we format our training data to capture the geometry of the detector.
The detector pad plane has 10,240 non-uniform pads that record data for 512 time steps per event, producing a resolution of 5,242,880 voxels in the detector volume. A feature vector of this length is not tractable for training our models. For logistic regression and fully-connected neural networks, we decrease our resolution to 8000 equal volume voxels by discretizing the $x$, $y$, and $z$ dimensions into 20 divisions each. Data was presented to the models as a one-dimensional vector of 8000 elements, where each element’s value represents the total charge recorded within that voxel’s boundaries. For CNNs, we created a two-dimensional projection in $x$ and $y$ and discretized that projection into 16,384 pixels, which can be represented by a $128 \times 128$ pixel image. In these images, the grayscale value is proportional to the total charge deposited onto the pads represented by each pixel. Some examples of the data presented to the CNN models are shown in Fig. 9.

4.4. Results

We now provide a brief overview of how the models described in Sec. 2 were implemented and tuned. We use the implementation of logistic regression from scikit-learn, an open-source machine learning library for Python [25]. This is an L2 regularized model, where the model parameters are determined using the SAG algorithm [26]. SAG is a variant of stochastic gradient descent that guarantees faster convergence by retaining some
Figure 9: A small subset of the training images for CNNs. The plots represent projections of the three-dimensional event data onto the $xy$-plane. The grayscale value indicates charge, where black is the highest charge and white represents no charge deposition. The simulated examples include added noise.

memory of past gradient updates. The logistic regression results presented in this section report the performance obtained using the best value of the regularization constant $\lambda$, as found by a grid search on a test-by-test basis.

For our fully-connected neural network models, we use an architecture with a single hidden layer, implemented using Keras, a high-level deep learning library written in Python [27]. Keras is a wrapper for TensorFlow, a software library for streamlined numerical computation and automatic differentiation that is widely used in machine learning applications [28]. The hidden layer in this model comprises 128 nodes and uses the ReLU activation function. We also employ dropout with a probability of 0.5 to prevent overfitting. The output layer uses either the sigmoid or the softmax activation function, depending on whether the learning task is binary or multi-class. The network weights are learned using the Adam optimization algorithm [29], a variant of stochastic gradient descent that uses an adaptive step size for
each parameter that depends on the magnitude of recent gradient updates. We use a learning rate of $10^{-5}$ and employ early stopping to determine the optimal number of training iterations.

The CNN models used in this work build atop the VGG16 model pre-trained on ImageNet [19]. As can be seen in Tab. 2, we found that starting with the preset VGG16 weights and fine-tuning the entire network using our datasets consistently outperformed using VGG16 simply as a feature extractor (using the approach described in Sec. 2.2.2). Thus, all our CNN results in the remainder of this section use the former approach. We replace the two fully-connected layers in the original VGG16 architecture with a single, smaller fully-connected layer comprising 256 units. We use dropout with a probability of 0.5 when training this layer. Our output layer is composed of either two sigmoid units or three softmax units, depending on whether the learning task is binary or multi-class, in place of the original 1000-unit output layer from VGG16. As with the fully-connected neural network models, we use Adam with a learning rate of $10^{-6}$ to tune the model parameters and use early stopping to determine the number of training epochs. Finally, we note that all models and code created for this project are accessible through the associated GitHub repository [30].

| learning type | task       | F1 score | Fine-tuning |
|---------------|------------|----------|-------------|
|               |            | Feature extraction | Fine-tuning |
| experimental  | binary     | 0.89     | 0.90        |
|               | multiclass | 0.88     | 0.93        |
| transfer      | binary     | 0.67     | 0.72        |
|               | multiclass | 0.65     | 0.67        |

Table 2: CNN model results: pre-trained CNN models were used as either fixed feature extractors, or were trained further starting from the preset weights. The resulting models were tested on experimental data. Fine-tuning the network outperformed feature extraction, and was thus used for all other CNN results presented.

4.4.1. Training and testing on simulated data

As noted earlier, training and testing on simulated data provides us with a useful upper-bound on how well we can expect our models to perform when they are evaluated on experimental data. Tab. 3 presents the results from the simulated data learning tasks using our three model families —
logistic regression (LR), fully-connected neural networks (FCNN) and fine-tuned convolutional neural networks (CNN). The results suggest that, given an ideal dataset, CNNs will perform best on the proton event classification task.

| algorithm | task      | noise | precision | recall | F1    |
|-----------|-----------|-------|-----------|--------|-------|
| LR        | binary    | no    | 0.59      | 0.32   | 0.41  |
|           |           | yes   | 0.57      | 0.29   | 0.38  |
|           | multiclass| no    | 0.61      | 0.46   | 0.52  |
|           |           | yes   | 0.61      | 0.45   | 0.51  |
| FCNN      | binary    | no    | 0.61      | 0.54   | 0.57  |
|           |           | yes   | 0.68      | 0.47   | 0.55  |
|           | multiclass| no    | 0.65      | 0.61   | 0.63  |
|           |           | yes   | 0.62      | 0.52   | 0.56  |
| CNN       | binary    | no    | 1.00      | 1.00   | 1.00  |
|           |           | yes   | 1.00      | 1.00   | 1.00  |
|           | multiclass| no    | 1.00      | 1.00   | 1.00  |
|           |           | yes   | 1.00      | 0.99   | 1.00  |

Table 3: Simulated data results: simulated data was used for training and testing each of our algorithms. The simulated data was also augmented with noise and retested to better understand how our model performance could be affected when applied to noisy events from the experimental data.

4.4.2. Training and testing on experimental data

Training and testing the models on experimental data requires manually labeling this data, which is not desirable in the analysis workflow. We are limited to much smaller training datasets in this setting when compared to the simulated data, which is also not ideal from a model-building standpoint. However, the results on this task help us identify the algorithms that succeed with our experimental data, which has noise signatures and events that we are unable to simulate in our synthetic datasets. These results are presented in Tab. 4 and, like the simulated data results in Tab. 3, suggest that the best algorithm for proton event classification is a CNN. While the workflow is not ideal, training on experimental data provides us with a classification model that is sufficiently successful to use in the analysis pipeline.
| Algorithm | Task   | Precision | Recall | F1   |
|-----------|--------|-----------|--------|------|
| LR        | Binary | 0.78      | 0.58   | 0.66 |
|           | Multiclass | 0.77    | 0.67   | 0.72 |
| FCNN      | Binary | 0.85      | 0.54   | 0.66 |
|           | Multiclass | 0.83    | 0.62   | 0.71 |
| CNN       | Binary | 0.98      | 0.84   | 0.90 |
|           | Multiclass | 0.96    | 0.90   | 0.93 |

Table 4: Experimental data results: these results were obtained by training and testing on hand-labeled data. The train and test sets came from a small dataset of fewer than 3000 events as reported in Tab. 1.

4.4.3. Transfer learning results

Successful transfer learning is the goal for this work, where the models are trained on simulated data and competently classify experimental data. This is ideal from an experimentalist’s perspective, as they do not have to manually label any data after the experiment has run. Tab. 5 reports our transfer learning results. As expected from our simulated and experimental results, CNNs performed the best at classifying proton scattering events in the experimental data, though the F1 scores have decreased significantly from the previous tests. This is expected since our simulated data does not perfectly model our experimental data.

4.4.4. Visualizing the learning results

In this section, we interrogate our fitted CNN model (trained on experimental data) to better understand how classification decisions are made. Specifically, we construct visual explanations of the model’s predictions using the Gradient-weighted Class Activation Mapping (Grad-CAM) algorithm [31]. Four representative examples are shown in Fig. 10. The top row in the figure shows the input images, while the heatmaps in the bottom row highlight the degree to which each region in an image contributed to the model’s overall decisions. The left-half of Fig. 10 presents cases where the model made correct predictions, on a proton event and an unknown event (arranged left-to-right). We see that the model’s “justification” for the proton classification arises from its focus on the spiral structure in that image, while its attention is more dispersed in the case of the unknown event. In the right-half of Fig. 10, we see cases where the model made incorrect predictions, namely a proton event mistakenly classified as non-proton, and a non-proton event...
Table 5: Transfer learning results: transfer learning is a more difficult learning problem, since the train and test data come from different distributions. Nevertheless, we see successful classification of proton scattering events using CNNs.

| algorithm | task  | noise | precision | recall | F1   |
|-----------|-------|-------|-----------|--------|------|
| LR        | binary| no    | 0.37      | 0.03   | 0.05 |
|           |       | yes   | 0.44      | 0.03   | 0.05 |
|           | multiclass | no    | 0.45      | 0.01   | 0.01 |
|           |       | yes   | 0.45      | 0.01   | 0.01 |
| FCNN      | binary| no    | 0.35      | 0.27   | 0.30 |
|           |       | yes   | 0.78      | 0.44   | 0.57 |
|           | multiclass | no    | 0.28      | 0.37   | 0.32 |
|           |       | yes   | 0.72      | 0.08   | 0.14 |
| CNN       | binary| no    | **0.90**  | **0.60** | **0.72** |
|           |       | yes   | 0.39      | 0.91   | 0.55 |
|           | multiclass | no    | 0.96      | 0.52   | 0.67 |
|           |       | yes   | 0.27      | 0.99   | 0.42 |

incorrectly classified as a proton (again arranged left-to-right). The model’s errors in these cases are understandable given the challenging identification task posed by these examples.

5. Conclusions

We found that machine learning methods are effective at identifying proton events in both simulated and actual AT-TPC data. Most significantly for experimentalists, we were able to construct models that could learn from artificial data and transfer this knowledge to actual data collected from the detector. The ability to train a model prior to conducting the physics experiment would allow automatic classification of events in real-time, with minimal need for human supervision. Further, such an approach could be easily adapted to other experiments, that utilize different instruments or detector technology, as all that is required is access to an accurate physics simulator.

Our highest performing model — a pre-trained convolutional neural network that was then fine-tuned for our domain — achieved an impressive precision of 0.90 on the transfer learning task. We note, however, that there
is still room for improvement, for this same model only has a recall of 0.60, for an F1 score of 0.72. In comparison, our best performing CNN model that also trained on experimental data was able to achieve an F1 score of 0.93. However, the latter approach comes at a cost: it requires laborious hand-labeling of a large batch of experimental data, before the classifier can be built. We believe that this performance gap can be closed with simulations that better capture the structural noise that is observed in experimental data — an avenue that we plan to pursue in future work.

6. Acknowledgements

This work supported in part by NSF grant no. 10049216 and the Davidson College Faculty Study and Research Grant.
References

[1] J. Bradt, D. Bazin, F. Abu-Nimeh, T. Ahn, Y. Ayyad, S. B. Novo, L. Carpenter, M. Cortesi, M. Kuchera, W. Lynch, W. Mittig, S. Rost, N. Watwood, J. Yurkon, Commissioning of the active-target time projection chamber, Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 875 (2017) 65–79.

[2] J. Bradt, Y. Ayyad, D. Bazin, W. Mittig, T. Ahn, S. B. Novo, B. Brown, L. Carpenter, M. Cortesi, M. Kuchera, W. Lynch, S. Rost, N. Watwood, J. Yurkon, J. Barney, U. Datta, J. Estee, A. Gillibert, J. Manfredi, P. Morfouace, D. Prez-Loureiro, E. Pollacco, J. Sammut, S. Sweany, Study of spectroscopic factors at N=29 using isobaric analogue resonances in inverse kinematics, Physics Letters B 778 (2018) 155 – 160.

[3] T. Hastie, R. Tibshirani, J. Friedman, The Elements of Statistical Learning: Data Mining, Inference and Prediction, Springer, second edition, 2009.

[4] C. Szegedy, S. Ioffe, V. Vanhoucke, A. A. Alemi, Inception-v4, inception-resnet and the impact of residual connections on learning, in: Proceedings of the Thirty-First AAAI Conference on Artificial Intelligence, February 4-9, 2017, San Francisco, California, USA., pp. 4278–4284.

[5] C. Chen, A. Seff, A. Kornhauser, J. Xiao, Deepdriving: Learning affordance for direct perception in autonomous driving, in: Proceedings of the 2015 IEEE International Conference on Computer Vision (ICCV), ICCV ’15, IEEE Computer Society, Washington, DC, USA, 2015, pp. 2722–2730.

[6] D. Silver, A. Huang, C. J. Maddison, A. Guez, L. Sifre, G. van den Driessche, J. Schrittwieser, I. Antonoglou, V. Panneershelvam, M. Lanctot, S. Dieleman, D. Grewe, J. Nham, N. Kalchbrenner, I. Sutskever, T. Lillicrap, M. Leach, K. Kavukcuoglu, T. Graepel, D. Hassabis, Mastering the game of go with deep neural networks and tree search, Nature 529 (2016) 484–503.

[7] B. Denby, Neural networks and cellular automata in experimental high energy physics, Computer Physics Communications 49 (1988) 429 – 448.
[8] G. Cybenko, Approximation by superpositions of a sigmoidal function, Mathematics of Control, Signals and Systems 2 (1989) 303–314.

[9] I. Goodfellow, Y. Bengio, A. Courville, Deep Learning, MIT Press, 2016. http://www.deeplearningbook.org

[10] D. E. Rumelhart, G. E. Hinton, R. J. Williams, Learning representations by back-propagating errors, in: J. A. Anderson, E. Rosenfeld (Eds.), Neurocomputing: Foundations of Research, MIT Press, Cambridge, MA, USA, 1988, pp. 696–699.

[11] Y. LeCun, B. Boser, J. S. Denker, D. Henderson, R. E. Howard, W. Hubbard, L. D. Jackel, Backpropagation applied to handwritten zip code recognition, Neural Comput. 1 (1989) 541–551.

[12] A. Krizhevsky, I. Sutskever, G. E. Hinton, Imagenet classification with deep convolutional neural networks, in: Proceedings of the 25th International Conference on Neural Information Processing Systems - Volume 1, NIPS ’12, Curran Associates Inc., USA, 2012, pp. 1097–1105.

[13] E. Shelhamer, J. Long, T. Darrell, Fully convolutional networks for semantic segmentation, IEEE Trans. Pattern Anal. Mach. Intell. 39 (2017) 640–651.

[14] A. Karpathy, L. Fei-Fei, Deep visual-semantic alignments for generating image descriptions, IEEE Trans. Pattern Anal. Mach. Intell. 39 (2017) 664–676.

[15] A. Aurisano, A. Radovic, D. Rocco, A. Himmel, M. Messier, E. Niner, G. Pawloski, F. Psihas, A. Sousa, P. Vahle, A convolutional neural network neutrino event classifier, Journal of Instrumentation 11 (2016) P09001.

[16] D. H. Hubel, T. N. Wiesel, Receptive fields, binocular interaction and functional architecture in the cat’s visual cortex, The Journal of Physiology 160 (1962) 106–154.

[17] V. Nair, G. E. Hinton, Rectified linear units improve restricted boltzmann machines, in: Proceedings of the 27th International Conference on International Conference on Machine Learning, ICML’10, Omnipress, USA, 2010, pp. 807–814.
[18] D. Scherer, A. Müller, S. Behnke, Evaluation of pooling operations in convolutional architectures for object recognition, in: Proceedings of the 20th International Conference on Artificial Neural Networks: Part III, ICANN’10, Springer-Verlag, Berlin, Heidelberg, 2010, pp. 92–101.

[19] K. Simonyan, A. Zisserman, Very deep convolutional networks for large-scale image recognition, CoRR abs/1409.1556 (2014).

[20] J. Deng, W. Dong, R. Socher, L. Li, K. Li, F. Li, Imagenet: A large-scale hierarchical image database, in: 2009 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR 2009), 20-25 June 2009, Miami, Florida, USA, pp. 248–255.

[21] J. Yosinski, J. Clune, Y. Bengio, H. Lipson, How transferable are features in deep neural networks?, in: Proceedings of the 27th International Conference on Neural Information Processing Systems - Volume 2, NIPS’14, MIT Press, Cambridge, MA, USA, 2014, pp. 3320–3328.

[22] N. Srivastava, G. Hinton, A. Krizhevsky, I. Sutskever, R. Salakhutdinov, Dropout: A simple way to prevent neural networks from overfitting, Journal of Machine Learning Research 15 (2014) 1929–1958.

[23] C. D. Manning, P. Raghavan, H. Schütze, Introduction to Information Retrieval, Cambridge University Press, New York, NY, USA, 2008.

[24] J. Bradt, Measurement of Isobaric Analogue Resonances of $^{47}$Ar with Active-Target Time Projection Chamber, Ph.D. thesis, Michigan State University, 2017.

[25] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, E. Duchesnay, Scikit-learn: Machine learning in Python, Journal of Machine Learning Research 12 (2011) 2825–2830.

[26] M. Schmidt, N. Le Roux, F. Bach, Minimizing finite sums with the stochastic average gradient, Math. Program. 162 (2017) 83–112.

[27] F. Chollet, et al., Keras, https://keras.io, 2015.
[28] M. Abadi, A. Agarwal, P. Barham, E. Brevdo, Z. Chen, C. Citro, G. S. Corrado, A. Davis, J. Dean, M. Devin, S. Ghemawat, I. Goodfellow, A. Harp, G. Irving, M. Isard, Y. Jia, R. Jozefowicz, L. Kaiser, M. Kudlur, J. Levenberg, D. Mané, R. Monga, S. Moore, D. Murray, C. Olah, M. Schuster, J. Shlens, B. Steiner, I. Sutskever, K. Talwar, P. Tucker, V. Vanhoucke, V. Vasudevan, F. Viégas, O. Vinyals, P. Warden, M. Wattenberg, M. Wicke, Y. Yu, X. Zheng, TensorFlow: Large-scale machine learning on heterogeneous systems, 2015. Software available from tensorflow.org.

[29] D. P. Kingma, J. Ba, Adam: A method for stochastic optimization, CoRR abs/1412.6980 (2014).

[30] J. Z. Taylor, attpc-event-classification, https://github.com/jtaylorz/attpc-event-classification, 2017.

[31] R. R. Selvaraju, M. Cogswell, A. Das, R. Vedantam, D. Parikh, D. Batra, Grad-CAM: Visual explanations from deep networks via gradient-based localization, in: IEEE International Conference on Computer Vision, ICCV 2017, Venice, Italy, October 22-29, 2017, IEEE Computer Society, 2017, pp. 618–626.