Machine Learning Applied to the Reionization History of the Universe in the 21 cm Signal

Paul La Plante\textsuperscript{1} and Michelle Ntampaka\textsuperscript{2,3}

\textsuperscript{1} Center for Particle Cosmology, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA; plaplant@sas.upenn.edu
\textsuperscript{2} Harvard-Smithsonian Center for Astrophysics, Harvard University, Cambridge, MA 02138, USA
\textsuperscript{3} Harvard Data Science Initiative, Harvard University, Cambridge, MA 02138, USA

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Abstract

The Epoch of Reionization (EoR) features a rich interplay between the first luminous sources and the low-density gas of the intergalactic medium (IGM), where photons from these sources ionize the IGM. There are currently few observational constraints on key observables related to the EoR, such as the midpoint and duration of reionization. Although upcoming observations of the 21 cm power spectrum with next-generation radio interferometers such as the Hydrogen Epoch of Reionization Array (HERA) and the Square Kilometre Array (SKA) are expected to provide information about the midpoint of reionization readily, extracting the duration from the power spectrum alone is a more difficult proposition. As an alternative method for extracting information about reionization, we present an application of convolutional neural networks (CNNs) to images of reionization. These images are two-dimensional in the plane of the sky, and extracted at a series of redshift values to generate “image cubes” that are qualitatively similar to those of the HERA and the SKA will generate in the near future. Additionally, we include the impact that the bright foreground signal from the the Milky Way imparts on such image cubes from interferometers, but do not include the noise induced from observations. We show that we are able to recover the duration of reionization $\Delta z$ to within 5\% using CNNs, assuming that the midpoint of reionization is already relatively well constrained. These results have exciting impacts for estimating $\tau$, the optical depth to the cosmic microwave background, which can help constrain other cosmological parameters.

Key words: cosmology: theory – dark ages, reionization, first stars – intergalactic medium – methods: numerical

1. Introduction

The Epoch of Reionization (EoR) is a portion of the universe’s history characterized by a large-scale phase change of the intergalactic medium (IGM) from neutral gas to ionized. The neutral hydrogen gas in the IGM emits radiation at radio frequencies with a wavelength of $\lambda = 21$ cm due to the hyperfine transition of the ground state, which is being pursued observationally through radio interferometer telescopes such as the Hydrogen Epoch of Reionization Array (HERA\textsuperscript{4}), the Low Frequency Array\textsuperscript{5}, and the Square Kilometre Array (SKA\textsuperscript{6}). These arrays seek to generate images of the EoR, which would provide insight into the topology of reionization and yield vital clues as to the astrophysical sources responsible for reionization. The images generated by these instruments can be useful for learning valuable information about these sources; for instance, locating highly ionized regions can pinpoint regions to perform follow-up analysis with other instruments such as the James Webb Space Telescope, or for cross-correlating with data from other surveys.

These images from the EoR can also be used to help constrain key properties of reionization, such as the midpoint and duration of reionization. However, extracting these parameters directly from the images may be challenging, due to the large degree of contamination from bright foreground emission from the the Milky Way. This emission is typically several orders of magnitude larger than the target signal, making simple imaging of the sky impossible. Due to their spectral smoothness, these foregrounds are mostly constrained to low $k_{\parallel}$-values in Fourier space. One approach for extracting information about reionization from such observations is to compute the power spectrum using Fourier modes that are uncontaminated by the foregrounds. Importantly, removing the $k_{\parallel} = 0$ mode precludes referencing an absolute scale, and so the resulting images are fluctuations about the mean temperature of the map rather than an absolute scale. However, such approaches do not leverage all of the information present in the images produced by these instruments. In particular, the power spectrum is insensitive to any non-Gaussian information present in the images. The 21 cm field is expected to be highly non-Gaussian during the EoR, and so there is valuable information that such approaches are potentially insensitive to.

An alternative approach to computing power spectra is to apply machine-learning techniques of image processing to simulated maps of the EoR. Such an approach allows for extracting non-Gaussian information present in the maps, without having to resort to explicitly computing higher-point statistics. We present here the use of convolutional neural networks (CNNs) to extract key features of the reionization history in seminumeric realizations of the EoR. In particular, we use CNNs to regress on the parameters of the midpoint of reionization $z_{50}$ and duration of reionization $\Delta z$. These two parameters are sufficient to characterize many of the key features of the reionization history, such as the optical depth to the cosmic microwave background (CMB) $\tau$. Constraining $\tau$ is useful in a broader cosmological context; providing tight priors on $\tau$ from observations of the EoR can yield smaller uncertainties on other cosmological parameters, specifically $A_s$, when analyzing CMB data (Liu et al. 2016).

\textsuperscript{4} https://reionization.org
\textsuperscript{5} https://www.lofar.org
\textsuperscript{6} https://www.skatelescope.org
Machine learning has been used in a variety of cosmological and astrophysical applications, including utilizing weak lensing beyond 2-point statistics to produce tighter cosmological parameter constraints (Gupta et al. 2018), parameter inference from weak lensing maps (Ribli et al. 2018), classifying reionization sources (Hassan et al. 2018), identify lensing signals in images (Lanusse et al. 2018), reducing errors in cluster dynamical mass measurements (Ntampaka et al. 2015), and morphological classification of galaxies (Dieleman et al. 2015). CNNs (e.g., Fukushima et al. 1982; LeCun et al. 1999; Krizhevsky et al. 2012) are a class of machine-learning algorithms that are typically used for image recognition and classification tasks. These networks are typically deep, utilizing many hidden layers to extract features from the input images by learning filters, weights, and biases to minimize a loss function on labeled training data. The authors of Gillet et al. (2018) have used CNNs to extract semianalytic reionization model parameters. This work builds on their findings, and demonstrates that information about the reionization history can be extracted even when accounting for some of the effects from observational foregrounds.

We organize the paper as follows. In Section 2, we describe the reionization model used and the method by which the input images are generated. In Section 3, we describe the machine-learning approach we employed. In Section 4, we present the results of our trained CNN and its ability to reconstruct the reionization history. In Section 5, we discuss provision of interpreting the intermediate output of CNNs. In Section 6, we conclude. Throughout the work, we employ a ΛCDM cosmology with cosmological constants given by the Planck 2015 results (Planck Collaboration et al. 2016).

2. Making Images of the EoR

The input to the CNNs discussed later are typically two-dimensional “images,” to which various mathematical functions such as convolutions are applied. Because the 21 cm field in principle provides a tomographic, fully three-dimensional picture of the universe as a function of wavelength/redshift, the input images must be converted to be two-dimensional by some method. In Gillet et al. (2018), the authors take one-dimension to be in the plane of the sky, and the other to be along the line-of-sight axis. This approach generates images of reionization “from the side,” in a sense, where the light cone-induced redshift evolution is explicitly presented to the CNN as one of the axes in the input images. However, actual images from interferometers in the near future will suffer from effects related to foreground contamination (Beardsley et al. 2015), and so this work endeavors to include a subset of such effects to investigate their impact on the ability of CNNs to extract useful information.

The approach presented in this work is to leverage the fact that CNNs can take multiple two-dimensional images as input. Each two-dimensional image is referred to as a “channel,” due to their typical usage of providing color information to CNNs in traditional image-recognition applications. As we outline in detail below, we generate a two-dimensional image of 21 cm signal in the plane of the sky, taking into account several foreground features imparted by interferometers. We generate images at multiple different redshifts, and pass each redshift image into the CNN as a separate channel. This approach results in input images that are more representative of what current and next-generation interferometers will be capable of than have been presented previously in the literature.

To provide input images to the CNNs discussed later, suitable images must first be generated representing reionization. To explore the effects of foreground contamination, we include several key instrumental effects, such as a finite angular resolution specific to HERA and the foreground wedge. We begin by discussing the semianalytic reionization model used in this project, then the observational effects included in the images, and finally how realizations were generated.

2.1. Reionization Model

The reionization model used in this work is based off of Battaglia et al. (2013b). It has been used to model the EoR (La Plante et al. 2014), and to understand the impact of patchy reionization on the kinetic Sunyaev-Zel’dovich (ksz) effect (Battaglia et al. 2013a; Natarajan et al. 2013). We summarize here some of the key features of the model, and refer to the other papers for a detailed discussion of the method.

The model of Battaglia et al. (2013b) assumes the "redshift of reionization field" \(z_{\text{re}}(x)\), defined as

\[
d(x) = \left[ \frac{z_{\text{re}}(x) + 1}{\bar{z} + 1} \right],
\]

is a biased tracer of the dark matter overdensity field

\[
d_m(x) = \frac{\rho_m(x) - \bar{\rho_m}}{\bar{\rho}_m}
\]

on large scales (>1 h⁻¹ Mpc). To quantify the precise relationship between the fields, a bias parameter \(b_{zm}(k)\) is introduced

\[
b_{zm}^2(k) \equiv \frac{\langle \delta_m^* \delta_z \rangle_k}{\langle \delta_m^* \delta_m \rangle_k} = \frac{P_z(k)}{P_m(k)}.
\]

We parameterize the bias parameter \(b_{zm}(k)\) as a function of spherical wavenumber \(k\) in the following way

\[
b_{zm} = \frac{b_0}{\left(1 + \frac{k}{k_0}\right)^\alpha}.
\]

The value \(b_0\) can be predicted using excursion set formalism in the limit \(k \to 0\) (Barkana & Loeb 2004). We use the value of \(b_0 = 0.593\). The reionization field for a given density field is then completely specified by the three values of the parameters \(\bar{z}\) in Equation (1), which determines the midpoint of reionization, and \(k_0\) and \(\alpha\) in Equation (4), which determine the duration.

An important feature to point out in the semianalytic model is that the redshift when the volume is 50% ionized \(z_{50}\) is in general not exactly equal to \(\bar{z}\) in Equation (1). This is due to the fact that the distribution of redshift values in the \(z_{50}(x)\) field are not symmetric about the mean, and so the median redshift is not equal to the mean. As such, throughout the rest of this paper, we will refer to the semianalytic model parameter as \(\bar{z}\) and the redshift when the volume is 50% ionized (by volume) as \(z_{50}\). Additionally, to quantify the duration of reionization \(\Delta z\), we compute the difference in redshift between when the volume is 25% ionized \(z_{25}\) and 75% ionized \(z_{75}\).
Mathematically,
\[
\Delta z \equiv z_{25} - z_{75}.
\] (5)

Other works have introduced parameters to quantify the asymmetry of reionization (Trac 2018), but for the current work we deal only with the midpoint and duration. These two numbers capture many of the physical reionization scenarios precipitated by Population II stars. So-called “exotic” reionization scenarios featuring Population III stars or mini-quasars are likely not accurately captured by this relatively simple seminumeric model of reionization, but we leave an investigation of these scenarios to future work.

2.2. Observational Effects

Mapmaking of the EoR using interferometers such as HERA or the SKA will include several interesting observational effects. First, the angular resolution of the instrument, determined by the longest baseline in the array, sets a lower limit on the spatial scales that can be probed by the instrument. Given a baseline vector connecting two interferometer elements \( b \), associated coordinates in the \( uv \)-plane are (Thompson et al. 2001)
\[
u = \frac{b}{\lambda},
\] (6)
where \( \lambda \) is the wavelength of the radiation of interest. For the redshifted 21 cm line, this is simply \( \lambda = \lambda_0 (1+z) \), with \( \lambda_0 = 21 \) cm. The \( uv \)-coordinates are related to the comoving wavenumber \( k_L \) in the plane of the sky through (Thyagarajan et al. 2015)
\[
\frac{k_L}{\lambda_c} = \frac{2\pi u}{D_c},
\] (7)
where \( D_c \) is the comoving distance along the line of sight to the observed redshift
\[
D_c(z) = c \int_0^z \frac{dz'}{H(z')},
\] (8)
where \( H(z) \) is the Hubble parameter. In general, an interferometer is not sensitive to information for Fourier modes with \( k_L > k_{L,\text{max}} \) defined by its largest baseline. For the fully constructed HERA-350 array, the longest baseline will be \( \sim 870 \) m (DeBoer et al. 2017). This corresponds to \( k_{L,\text{max}} \sim 0.5 \) h\(^{-1}\) Mpc at \( z = 8 \). To generate images that reflect this limited angular resolution, we apply a mask in Fourier space where the value of all modes is set to 0 where \( k_L > k_{L,\text{max}} \) (discussed below in detail in Section 2.3).

Another more subtle observational effect is the impact that the aforementioned smooth foregrounds have on the signal. The dominant signal in the radio portion of the electromagnetic spectrum at these wavelengths is “foreground” emission from our own the Milky Way. Specifically, the galactic synchrotron radiation has a brightness temperature of several thousand Kelvin at 150 MHz. Because synchrotron radiation follows a power law as a function of frequency, it is very smooth in Fourier space. Naively, all of the power from these foregrounds would fall into bins of small values of \( k_L \).

Unfortunately, due to the chromaticity of an interferometer, the power from these small-\( k_L \) modes scatters to higher values of \( k_L \). For an explanation of why this happens, see Parsons et al. (2012). The amount of contamination is a function of \( k_L \), and increases sharply as \( k_L \) increases. The resulting foreground contamination is affectionately referred to as “the wedge” in the literature (Datta et al. 2010; Morales et al. 2012; Vedantham et al. 2012; Liu et al. 2014). The slope of the wedge \( m \) in \( k_L \)-space is largely independent of the specifics of the instrument, and can be written as (Thyagarajan et al. 2015)
\[
m(z) \equiv \frac{k_L}{\lambda_c} = \frac{\lambda D_v f_{21} H}{c^2 (1+z)^2},
\] (9)
where \( \lambda = \lambda_0 (1+z) \) is the wavelength of the 21 cm signal at the redshift of interest, \( D_v \) is the comoving distance to a redshift \( z, f_{21} \) is the rest-frame frequency of the 21 cm signal, and \( H \) is the Hubble parameter of redshift \( z \). For the redshifts of interest, \( m \sim 3 \). In this expression, we have assumed the maximal horizon contamination; physically, the bright foreground contamination extends down to the horizon of the interferometer beam. In practice, with foreground mitigation and removal schemes, the slope of the wedge may not be as steep as the expression in Equation (9). If the contamination is not as dire as that specified by Equation (9), then the accuracy of the predictions should only increase, because there is more information available to the CNN in the input images during training. Conversely, if more modes are contaminated than those which naively should be foreground-free, the resulting images of the EoR from interferometers such as HERA may in fact be worse than those presented here. The quality of actual images will depend on the processing details of mapmaking using the visibility data, and so future studies may require a more nuanced treatment of foreground contamination.

2.3. EoR Input Image Generation

To actually construct the reionization realizations used as input images, we first perform an \( N \)-body simulation to generate the dark matter density field \( \delta_m \) used in Equation (2). The \( N \)-body simulation uses a \( \text{P}^3\text{M} \) algorithm described in Trac et al. (2015), and contains \( 2048^3 \) dark matter particles in a volume of \( 2 \) h\(^{-1}\) Gpc on a side. At regularly spaced intervals in redshift, the particles are deposited on a grid using a cloud-in-cell (CIC) scheme onto a uniform grid of \( 2048^3 \) resolution elements. In order to obtain the density field at an arbitrary redshift, the two neighboring matter density fields are loaded into memory, and interpolated in scalefactor \( a \) for every point in the volume. This allows for the construction of an approximate density field for any desired redshift without having to run a new simulation ab initio.

To generate a new series of input images, a new set of model parameters \( \{ \bar{z}, k_0, \alpha \} \) are chosen. The density field \( \delta_m(\bar{z}) \) is generated for the mean redshift \( \bar{z} \), according to the scheme described in the previous paragraph. Then, the density field is Fourier transformed into \( k \)-space to generate \( \delta_m(\mathbf{k}) \), and the bias relation defined in Equation (4) is applied as a function of

\footnote{The foreground contamination actually extends slightly beyond the horizon limit. This “supra-horizon buffer” is due to the intrinsic spectral unsmoothness of the foreground signal (Pober et al. 2013). The amount of additional leakage is relatively small, especially for the longest baselines, which are most important for forming images.}
spherical wavenumber $k$ to generate $\delta_c(k)$. The field is inverse Fourier transformed to arrive at $\delta_c(x)$, and Equation (1) is inverted to get the field $z_{\text{re}}(x)$. This field encodes the entire reionization history for the volume given the density field and model parameters chosen.

As discussed in Section 2, the next task is to generate the 21 cm field $T_{21}$ at a fixed series of redshifts, and apply the foreground effects described in Section 2.2. This process generates input images that attempt to be representative of images generated by HERA in the next 2–3 yr–images from a next-generation experiment, such as the SKA, which will presumably provide images with even higher sensitivity and fidelity. Given a snapshot $i$ with redshift $z_i$, the matter density field is generated by interpolating using bracketing redshifts as described earlier to generate $\delta_m(x, z_i)$. The 21 cm brightness temperature field $\delta T_b$ corresponding to this redshift is then generated by using the formula (Madau et al. 1997)

$$\delta T_b = 26(1 + \delta_m)x_{\text{HI}}\left(\frac{T_S - T_i}{T_S}\right)\left(\frac{\Omega_m h^2}{0.022}\right) \times \left[\frac{0.143}{\Omega_m h^2}\left(\frac{1 + z}{10}\right)\right]^2 \text{mK},$$

(10)

where $x_{\text{HI}}$ is the neutral fraction field for a given point in the volume, $T_S$ is the spin temperature of the gas, and $T_i$ is the temperature of the CMB at redshift $z_i$. For simplicity, we assume that the ionization field only takes on values of 0 (for a totally ionized part of the volume) or 1 (for a neutral region). In particular, if $z_{\text{re}}(x) < z_i$, then the model predicts a later redshift of reionization than the redshift in question, and so that part of the volume is neutral. Also, we assume that the spin temperature is much greater than the CMB temperature, so $(T_S - T_i)/T_S \rightarrow 1$. This assumption is valid once the spin temperature is coupled to the kinetic temperature of the gas, which happens once the gas is ionized at the ~25% level (Santós et al. 2008). As shown by Greig & Mesinger (2017), incorrectly assuming spin temperature saturation can bias the recovery of semianalytic model parameters, especially when applied at high redshift ($z \gtrsim 15$) when the spin temperature is not saturated. Because we are interested in extracting the timing of the midpoint and central duration of reionization, the assumption of spin temperature saturation was used in the application at hand. It should be noted, though, that this model is overly naïve for understanding how the brightness temperature behaves at the very onset of reionization, and may be inaccurate for the highest redshift layers in our input images ($z \sim 12$). A more detailed treatment of the spin temperature should be used if applying this technique to simulated images of the pre-reionization epoch.

Once a new reionization history has been generated given the model parameters $\{z, \alpha, k_{\phi}\}$, a series of snapshot images are generated. To avoid biasing the results of the CNN by tracing out the same density structure with different reionization histories, starting indices $(i, j, k)$ are chosen randomly, as well as a random line of sight along the $x$-, $y$-, or $z$-axis. Starting at these coordinates, a series of 20 snapshots spanning the range $5.5 \leq z \leq 12$ are chosen along the line of sight, evenly divided in comoving distance. At a given redshift snapshot $z_i$, a two-dimensional slab is generated, with the axes in the plane of the sky spanning the full size of the simulation volume (2 $h^{-1}$ Gpc $\times$ 2 $h^{-1}$ Gpc) and the axis along the line of sight spanning $\sim 48.8$ $h^{-1}$ Mpc. The redshift evolution along this distance is small enough so the slab can be approximately considered comoving, and so there is no light cone effect induced (La Plante et al. 2014). This slab is then Fourier transformed, and Equations (7) and (9) are applied (the maximum angular resolution observable for HERA and the effect of foreground contamination, respectively). Specifically, all Fourier modes where $k_i > k_{\text{max}}$ for HERA are removed, as well as all modes for which $k_i \leq mk_i$. Additionally, to reduce the final size of the output images, we downselect to the smallest $N/4$ Fourier modes along the $k_i$ axes. With these observational effects applied, we inverse Fourier transform, and then select the central slice of this slab. This approach roughly approximates performing a narrow-band measurement of the interferometer, though the impact of thermal noise has been neglected. Its impact can be fairly significant for different interferometer designs (Hassan et al. 2018), but for this initial analysis we ignore its effect.

Having generated a series of 20 redshift snapshots in the above manner (which results in an array with dimensions of $512 \times 512 \times 20$ pixels), the result is saved as a single “image” to be used for training the CNN and evaluating its performance. The axis of evolution along redshift is treated as different “color channels” in the CNN architecture. Additionally, the reionization history is computed, and the midpoint and duration are saved. These values will serve as the “labels” when training the CNN. Altogether, we generate 1000 of these images to use for training and testing purposes. In the analysis that follows, we keep $\bar{z}$ fixed, and allow the other reionization model parameters $\alpha$ and $k_{\phi}$ to vary, effectively changing the duration of reionization while keeping the midpoint nearly constant. This type of analysis could apply if the midpoint of reionization were derived from, e.g., power spectrum analysis (Lidz et al. 2006), but with the duration being relatively unconstrained. In future analysis, we plan to extend this work to regress on the duration and midpoint simultaneously, which would help serve as an independent confirmation of the reionization history derived from other methods.

Figure 1 shows a side-by-side comparison of a typical “image” (20 redshift layers which serve as a single input image to the CNN), both with and without the instrumental effects discussed in Section 2.2. Notably, the zero-level of the image is adjusted when the foreground effects are applied and the $k_i = 0$ modes are removed. In essence, the bottom row of Figure 1 shows just the dynamic range of the images, rather than an absolutely referenced scale of the signal, as seen in the top row. In other words, although the reionization history is encoded in the sky-averaged global signal of the redshifted 21 cm line, this information is not presented to the CNN trained as part of the analysis—the CNN only ever receives images like the bottom row as “input.” Also, the features in the images shift once the foreground effects are applied, due to the cuts made in Fourier space. Also note that the features generally become blurrier and less well resolved, an effect of the finite resolution of HERA.
3. Machine-learning Techniques

CNNs (e.g., Fukushima et al. 1982; LeCun et al. 1999; Krizhevsky et al. 2012) are a class of feed-forward machine-learning algorithms commonly used in image recognition tasks. They employ a deep network with hidden layers, and require very little preprocessing of the input images because the network learns the convolutional filters necessary to extract relevant features for classification or regression tasks.

The architecture of the our CNN is shown in Figure 2 and is based loosely on the architecture of Simonyan & Zisserman (2014), but with fewer hidden layers. Feature extraction is performed with three convolutional and pooling layers. The convolutional layers use $3 \times 3$ convolutional filters, and are coupled with $2 \times 2$ max pooling layers with a stride of 2 (e.g., Riesenhuber & Poggio 1999). In between the convolutional and max pooling layers, a batch normalization layer is used to provide regularization (Ioffe & Szegedy 2015). Following feature extraction, regression is performed by three hidden, fully connected layers. The fully connected layers employ rectified linear unit (Nair & Hinton 2010) activation. A 20% dropout after each fully connected layer is used to prevent overfitting (Srivastava et al. 2014).

The full architecture is as follows:

1. $3 \times 3$ convolutional layer with 16 filters
2. batch normalization
3. $2 \times 2$ max pooling layer
4. $3 \times 3$ convolutional layer with 32 filters
5. batch normalization

Figure 1. Visualization of the 21 cm images before (top) and after (bottom) the application of the foreground effects described in Section 2.2. The different columns are different redshift slices, with the redshift shown on the image. The most dramatic change is that the zero-level is no longer the absence of the 21 cm signal, as in the top row, but the mean value of the Fourier transformed slab. This effect is due to the removal of the $k_0 = 0$ mode as part of the foreground effects, which ensures that the resulting inverse Fourier transformed slab must have mean 0. Also note that the structures in the top panel are no longer in the corresponding places in the bottom panel, another effect of the application of the foreground wedge. Although this effect makes matching the locations of individual sources difficult, statistically, the fields seem to have similar properties. See Section 2.3 for more discussion.

Figure 2. Visualization of the CNN architecture used in the analysis. The input images are $512 \times 512 \times 20$, and the output is two meta-parameters $z_{50}$ and $\Delta z$ quantifying the midpoint and duration of reionization, respectively. As shown in the figure, there are many hidden layers between the input and output. The addition of hidden layers has been shown to increase the efficacy of the network in processing image-like data (Schmidhuber 2014). See Section 3 for a detailed description of the full architecture of the network.
6. 2 × 2 max pooling layer
7. 3 × 3 convolutional layer with 64 filters
8. batch normalization
9. 2 × 2 max pooling layer
10. global average pooling layer
11. 20% dropout
12. 200 neuron fully connected layer
13. 20% dropout
14. 100 neuron fully connected layer
15. 20% dropout
16. 20 neuron fully connected layer
17. output neurons

See also Schmidhuber (2014) and references therein for a review of deep neural networks.

We perform a fivefold cross validation, cyclically training on 80% of the images, and reporting the results of the remaining 20%. Each model is trained for 200 epochs and trains to minimize a root mean squared error (RMSE) loss function. The CNN architecture described above is implemented using the Keras package (Chollet 2015), with the TensorFlow package (Abadi et al. 2016) providing the backend computation engine to take advantage of GPU processing. Also, by construction all images in the training set had the same mean redshift of reionization $\bar{z} = 8$; however, as discussed above in Section 2.1, the midpoint of reionization $z_{50}$ was not identically the same as $\bar{z}$, and varied from $7.7 \lesssim z_{50} \lesssim 7.9$. Empirically, better results were achieved by training the CNN to regress on both the midpoint and duration, and we present results for both parameters below.

Figures 3 and 4 show the loss as a function of epoch. The solid lines show the loss for the training set and the dashed lines are the loss for the test set. The oscillations in the test set decrease significantly after the first ~25 epochs, showing that the majority of the “learning” happens during this initial set of epochs. Afterwards, the small disparity between the training and test set loss values demonstrates that the CNN is not overfitting the training set. The fact that the loss is generally decreasing for all epochs shows that the network is converging on a solution. Although some of the folds seem to have converged before 200 epochs, the loss does not increase, meaning the networks have not overfitted the data.

4. Results

As discussed in Section 3, the CNNs were trained by minimizing the RMSE of the predicted reionization parameters relative to the true ones. Here we present the results of predicting the midpoint $z_{50}$ and duration of reionization $\Delta z$. Note that both the midpoint and duration were used as output “prediction” neurons, and were regressed on as part of the RMSE loss function.

Figure 5 shows the output of the CNN regression for the midpoint of reionization $z_{50}$. As discussed in Section 3, the CNN produces estimates of both $z_{50}$ and $\Delta z$ for the input images, despite the fact that $z_{50}$ remained relatively constrained for the different input images. For most of the folds, the trained...
network is able to recover the input value of \( z_{50} \) highly accurately, with errors much less than 1%. However, for Folds 1 and 2, the output values are biased low for high values of \( z_{50} \). This is likely due to the relatively large gaps in between the central redshifts of the input layers. The gap in redshift between adjacent layers \( \tilde{z} \) is typically \( \tilde{z} \sim 0.3 \), which can make very precise prediction of the midpoint difficult. Decreasing the spacing between adjacent redshift snapshots should help eliminate the bias, though the accuracy of the current results is still quite good.

Figure 6 shows the output of the CNN regression for the duration of reionization \( \Delta z \). The top panel of Figure 6 shows the absolute deviation from the correct value, and the lower panel shows the relative deviation of the value of \( \Delta z \). As can be seen in the lower panel, the variation is typically \( \pm 5\% \) or smaller, implying that the CNN trained using the input data can predict the duration of reionization reasonably well. As with some of the folds in Figure 5, some of the folds show a biased result that changes as a function of the true value of \( \Delta z \). Interestingly, this bias tends not to be consistently positive or negative for all values of \( \Delta z \). As with the bias in Figure 5, the bias is likely due to the relatively large spaces in redshift space between adjacent snapshots. Decreasing this spacing may increase the accuracy of the ultimate predictions.

The results in Figure 6 show that the CNN is able to accurately predict the duration of reionization from a single \( 512 \times 512 \times 20 \) input image to the CNN. Given the field of view of HERA and its observation strategy, it is expected to generate a modest number (10–20) of such independent observations. Assuming that statistical errors dominate the uncertainty over systematic errors, the ultimate accuracy with which HERA would be able to constrain the duration of reionization \( \Delta z \) should be even better than the 5% shown in the figure. Part of this extrapolation assumes that the duration of reionization is well-characterized by the semianalytic model used in this analysis, and so in future work we plan to use additional semianalytic tools, such as 21CMFAST (Mesinger et al. 2011) to test whether the results are robust when using a different semianalytic model. As discussed in Section 2.2, we also plan to incorporate the effect of thermal noise from interferometer measurements in future analysis.

5. Discussion

Gaining physical insight from deep networks is difficult, but not impossible. CNNs are often utilized as a black box that takes an unprocessed image as an input and outputs an image label, but this need not be the case. Filter visualization is one way to interpret these systems to add a human layer of interpretability and physical understanding to the tool.

Motivated by the work in Chollet (2016) to visualize filters of an image classifier, we explore the types of input images that maximize neurons of the global average pooling layer. This type of analysis is useful for understanding the types of images that the CNN has been trained to interpret, and can be useful for seeing which types of features are most important to the CNN. Other approaches to visualizing “what the CNN sees,” such as passing the input images through one or several convolutional layers, can be useful for understanding how the images are modified as they pass through the series of convolutional filters. However, they do not necessarily show which features in particular the network is responding to. The reason for this is that those types of analysis rely on permuting some typical input, rather than allowing the input images to maximize the response of a given neuron deep in the network. Though the visualization approaches are related, they are fundamentally showing different aspects of the CNN learning process.

We create an input image that is the same size \( (512 \times 512 \times 20) \) as one training image. These images are initially white noise; for each of the 20 redshift slices, the pixels are populated by random numbers that span a typical pixel value range of the input data at that redshift. Through the iterative process described in detail in Chollet (2016), the pixel values of these noisy input images are altered through gradient ascent over 10 iterations to maximize the response at the global max pooling layer.

After each iteration, we employ a normalization to prevent single pixels from dominating the effect as well as a smoothing to make the resulting images easier to visually interpret. The normalization is achieved simply by multiplying each pixel value by 0.8 to minimize very bright pixels. The smoothing is accomplished with a Gaussian blur with \( \sigma = 5 \) pixels that extends along the \( 512 \times 512 \) single-redshift image but does not blur one redshift slice into another.

A sample of these images is shown in Figure 7. This visualization shows the input images that maximize the response to eight different nodes deep in the CNN, for the same redshift layer (one corresponding to \( z \approx 5.8 \)). Interestingly, the shapes and patterns for a given node do not vary significantly across the different redshift layers. This behavior suggests that each neuron is responding to a particular pattern in the input data at different redshifts, though the relative importance between these patterns can change by changing the weights. We have selected several of the typical patterns seen for the different nodes, which represent nearly all of the different ones seen in the various filters. We may be able to ascribe some physical interpretation to the different patterns, which will help in understanding which trends are most important to the CNN when regressing on the duration of reionization.

The first few filters on the left side of the figure show, broadly, variations in the large-scale structure present in the input maps. The input images to the CNN represent comoving volumes that are \( 2 h^{-1} \) Gpc in size, and so these large-scale fluctuations are tens to hundreds of Mpc on a side. Rather than
detecting individual ionized regions, these filters seem to be picking up on the large-scale contrast present in the maps. The size of the connected regions can also change, and seem to range from large scales to intermediate scales, and finally relatively small scales. Additionally, the dynamic range and sign of the contrast can change for the different scales. Of the 64 output neurons from this layer, 8 of the “typical” output patterns are presented. The different filters seem to be keying in on different features in the images: the patterns on the left describe large-scale differences in the patterns of the input images, whereas the ones on the right identify small-scale contrast. See Section 5 for additional comments.

In the two rightmost panels of Figure 7, there are two input images that focus on the small-scale contrast of the input images. However, there is a distinct difference in the shape of this small-scale structure: one has more circular features, and the other has elliptical ones. This may be a reflection of the CNN using the degree of anisotropy of the small-scale structure as a way of determining the duration of reionization. As seen in Figure 4 of La Plante et al. (2014), shorter reionization scenarios tended to have more anisotropic features compared to longer reionization histories. Though this may be a feature of the common semianalytic model used in both works, it nevertheless points to an interesting feature that the CNN may be using to determine the reionization history. More generally, the degree of anisotropy in the 21 cm maps may hint at the relative bias of the luminous sources contributing to reionization. If these types of features are present in similar analysis employed by other semianalytic models of reionization, it may point to a common underlying physical property being used by the CNN. We plan to pursue such comparisons in future work.

6. Conclusion

In this work, we show that we are able to train a CNN to accurately predict the duration of the EoR to 5% or better. The input images for this task have been modified to reflect some of the effects that foreground avoidance and removal strategies in HERA data processing are expected to impart to real-world images generated in the next few years, though the inclusion of thermal noise is saved for future work. We show that despite the degradation in input image quality, the CNN is able to extract the target parameter with reasonable accuracy. The ultimate accuracy of such a method will be improved by combining independent image cubes generated from statistically independent portions of the sky. Constraining the duration of reionization with a relatively high degree of accuracy has exciting implications on the ability to provide priors on τ, the optical depth to the CMB. Such a constraint can be used to decrease the uncertainty of other cosmological parameters, such as A_S, which are partially degenerate with τ.

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ORCID iDs

Paul La Plante @ https://orcid.org/0000-0002-4693-0102
Michelle Ntampaka @ https://orcid.org/0000-0002-0144-387X

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