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Lecture 15
Signal Emulation for Astrophysics and Cosmology

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Overview

- Why we need signal emulators?
- Example of a 21-cm signal emulator
- Example Dimensionality Reduction
- Brief discussion of CNNs for SKA power spectrum measurements

Slides available at https://github.com/htjb/Talks (and Moodle!)

Example codes on github too!

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Why we need signal emulators?

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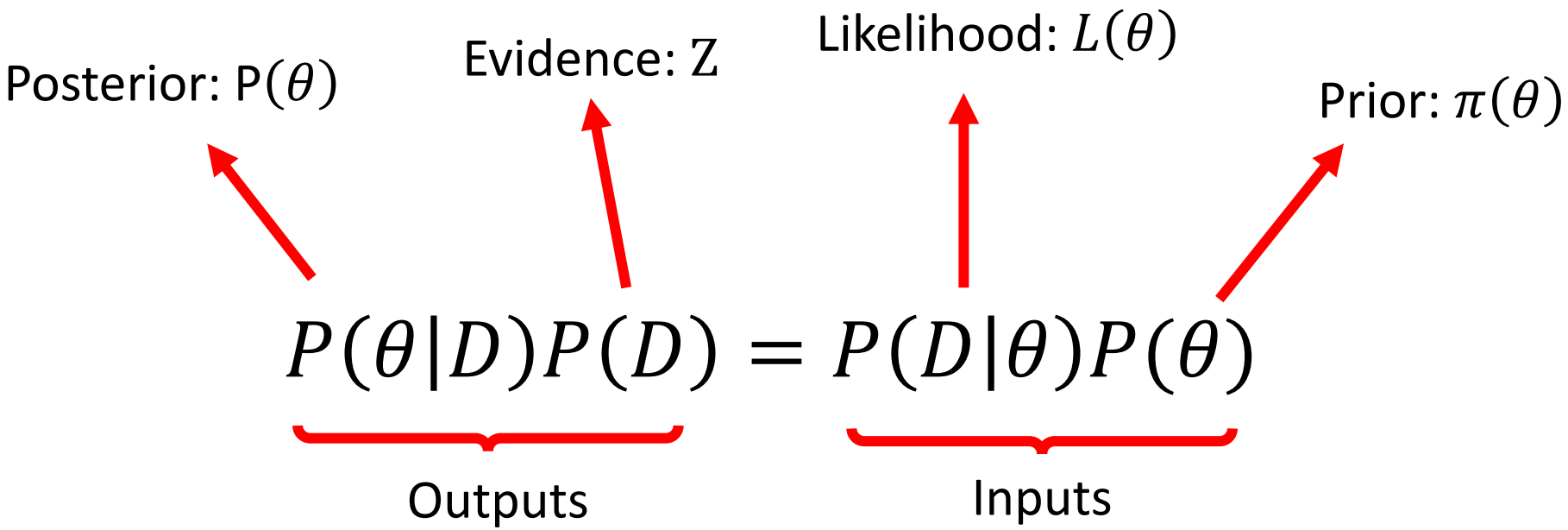
Recap:Bayes theorem



For MCMC or Nested Sampling

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The likelihood function

- The likelihood function gives the probability of the *data given the model and parameters* $L(\theta) = P(D|\theta, M)$
- Defined as an input to Nested Sampling or MCMC algorithms
- A lot of research goes into the form of the likelihood which varies for different analysis problems (e.g. Scheutwinkel et al. 2023 https://arxiv.org/abs/2204.04491)

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An example likelihood

$$\log_e L(\theta) = \sum_i -\frac{1}{2}\log_e 2\pi|\Sigma| - \frac{1}{2}\left(D_i - M_i(\theta)\right)^T \Sigma^{-1}(D_i - M_i(\theta))$$

- Work in log space to make things more computationally stable
- The functional form of the likelihood defines the noise distribution in your data
- Here we are assuming the noise is Gaussian and allowing for a non-diagonal covariance

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The issue

$$\log_e L(\theta) = \sum_i -\frac{1}{2}\log_e 2\pi|\Sigma| - \frac{1}{2}\left(D_i - M_i(\theta)\right)^T \Sigma^{-1}(D_i - M_i(\theta))$$

- In a Nested Sampling run or MCMC the likelihood function is evaluated for different θ hundreds of thousands to millions of times
- This means we need to evaluate the model $M(\theta)$ millions of times
- But the models are often computationally expensive taking minutes to hours to days per realization

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The issue

$$\log_e L(\theta) = \sum_i -\frac{1}{2}\log_e 2\pi|\Sigma| - \frac{1}{2}\left(D_i - M_i(\theta)\right)^T \Sigma^{-1}(D_i - M_i(\theta))$$

- How do we get around this?
- Look towards emulators which can approximate $M(\theta)$ in less than a few milliseconds
- Go from millions or hours to hours per Nested Sampling/MCMC run

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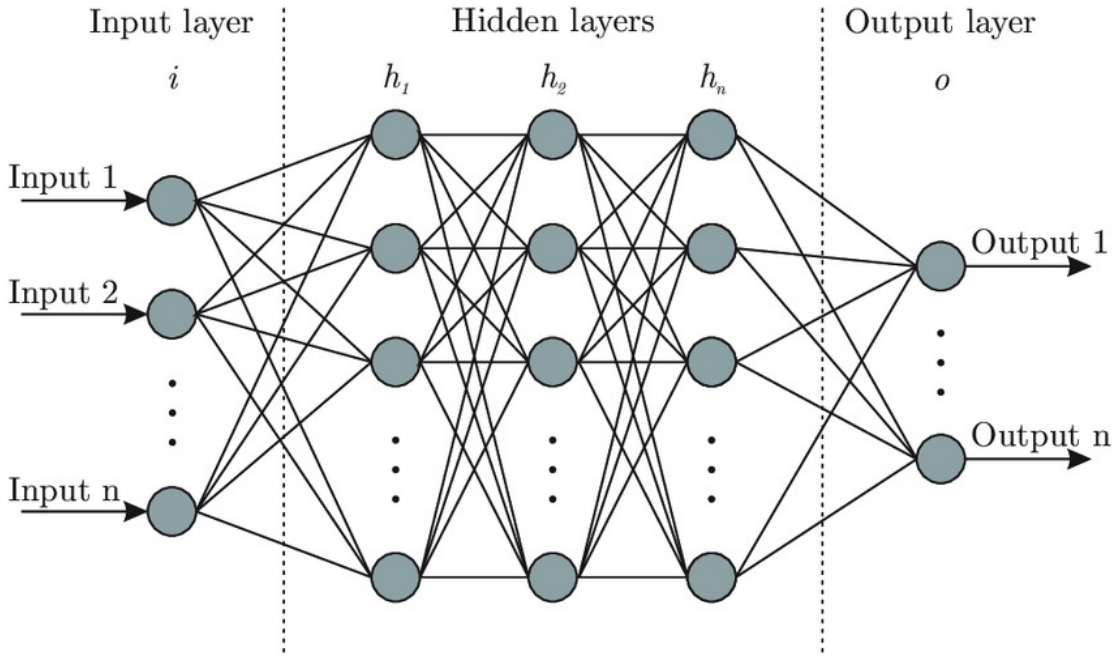
What actually is an emulator?

- Some approximation of a complex astrophysical model (think N-body, hydrodynamical or semi-numerical simulations)
- Often built with machine learning tools
- Artificial neural networks and Convolutional neural networks



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Sky-averaged 21-cm Cosmology

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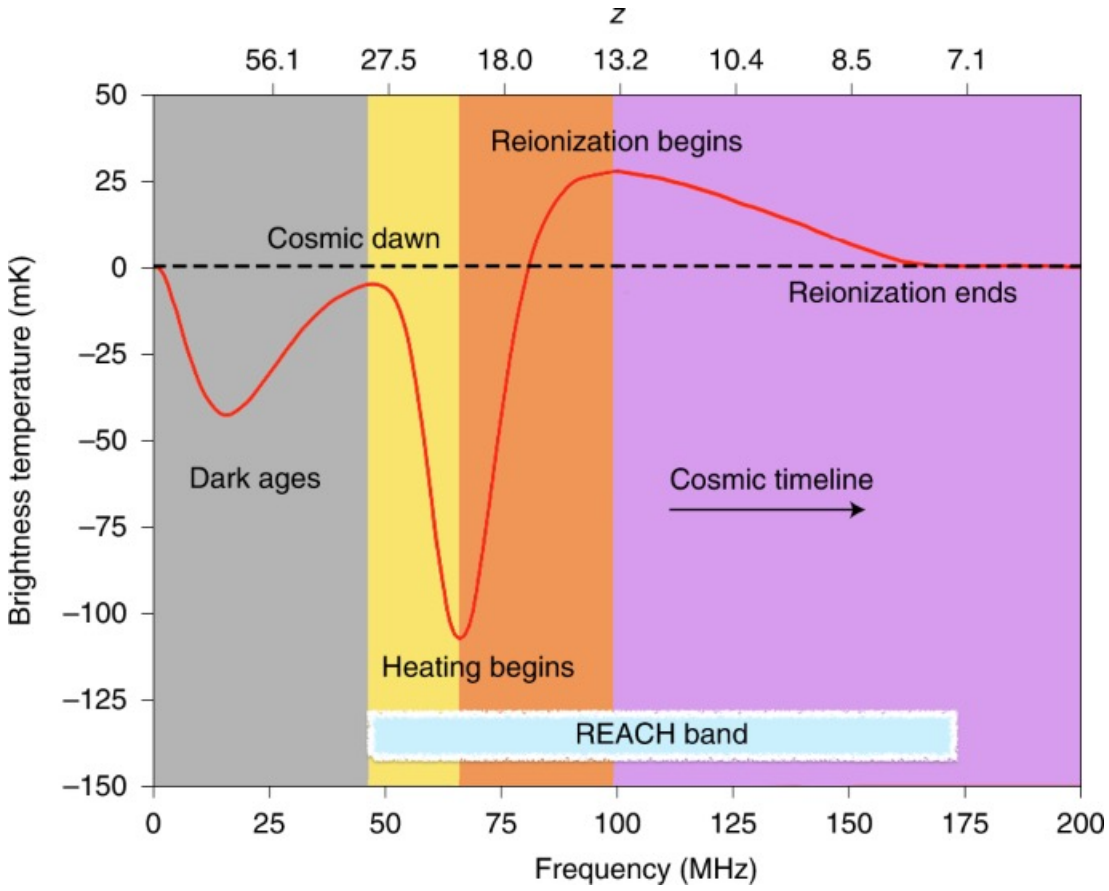
Sky averaged 21-cm Cosmology

- Looking for a spectral distortion in the CMB temperature caused by neutral hydrogen
- A detection of the signal will help us understand
  - When the first stars formed ad how bright they were
  - The nature of dark matter
  - The abundance and brightness of X-ray emitting objects
  - When the universe transformed from neutral to ionized



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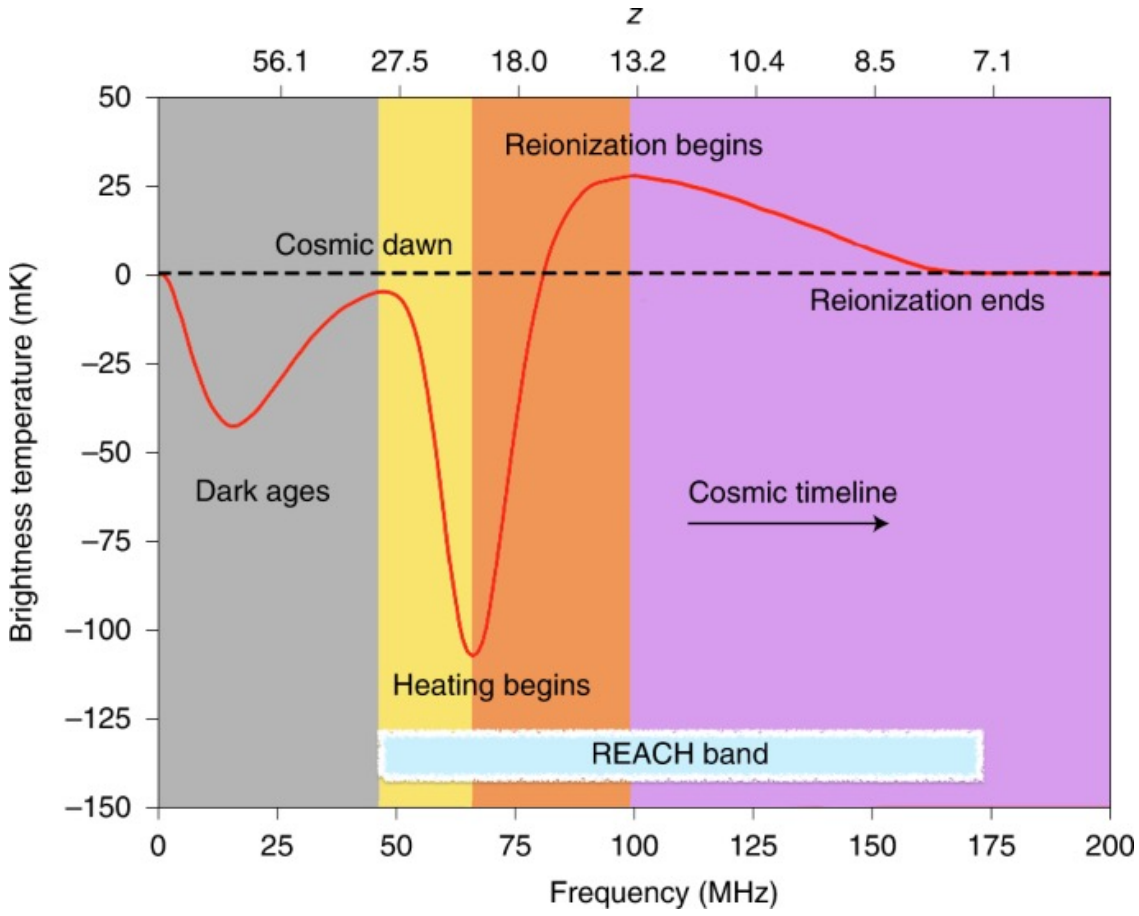
Sky averaged 21-cm Cosmology

- Complex dependence between T_{21} and the parameters of our models θ
- We use semi-numerical simulations to model and study how the signal varies over space and time for given θ
- One signal realization takes $\approx$ 3hrs



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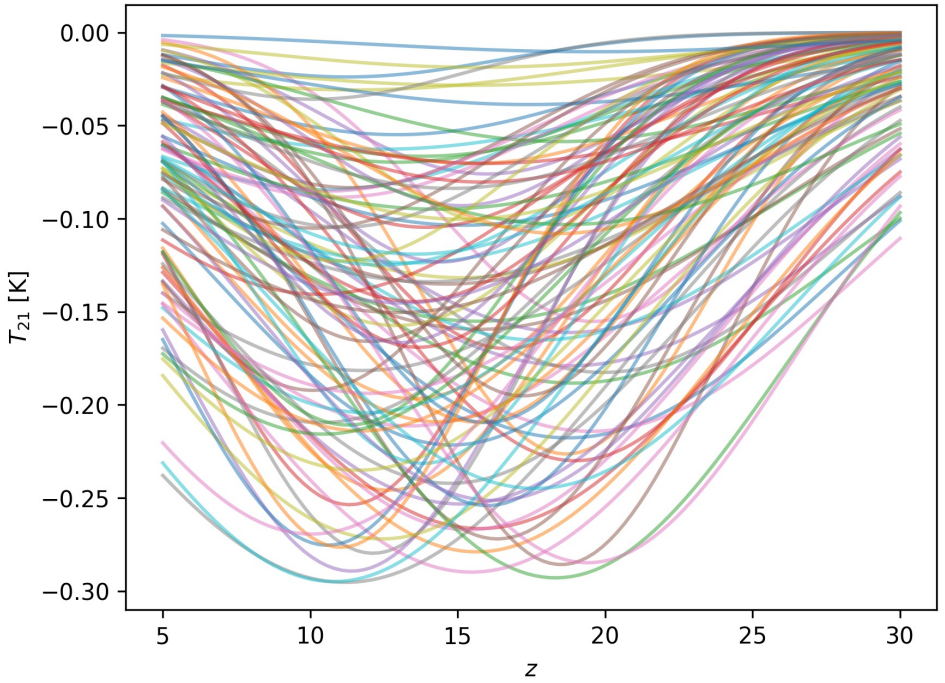
A toy 21-cm Cosmology example

- We can approximate the 21-cm signal with a Gaussian absorption feature

- Parameterised by
  - An amplitude A
  - A width σ
  - A central redshift z_c

- We want to approximate the simulation with a neural network $\mathrm{T}_{21}(\theta) \approx f_{\phi}(\theta)$

```
def gaussian(parameters):
    """a simple Gaussian function"""
    return -parameters[0] * \
        np.exp(-0.5*(z - parameters[1])**2/
               parameters[2]**2)
```



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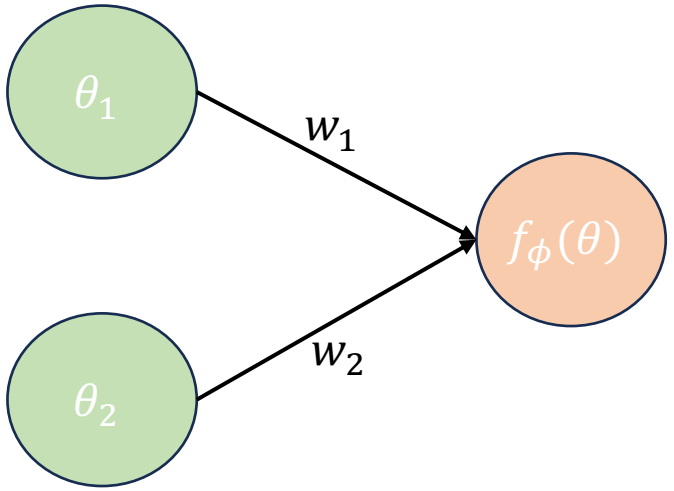
Emulators as an approximation

- In $\mathrm{T}_{21}(\theta) \approx f_{\phi}(\theta)$, ϕ are the parameters of our neural network
- ϕ has to be optimized so that the approximation is accurate as possible
- Can say $\mathrm{T}_{21}(\theta) = f_{\phi}(\theta) + \epsilon_{\phi}(\theta)$ where we are attempting to minimize the error $\epsilon_{\phi}(\theta)$



$$f_\phi(\theta) = \sigma(w_1\theta_1 + w_2\theta_2)$$

where

$$\phi = \{w_1, w_2\}$$

and σ is an activation function

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Loss Function

- In order to minimize the error $\epsilon_\phi(\theta)$ we have to provide the network with training data $\{T_{21}, \theta\}$

- For each example we evaluate some measure of error e.g.

$$L = \frac{1}{N}\sum_i \left|\epsilon_\phi(\theta)\right| \text{ or } L = \frac{1}{N}\sum_i \left(\epsilon_\phi\right)^2$$

- And adjust ϕ using Stochastic Gradient descent to minimize L

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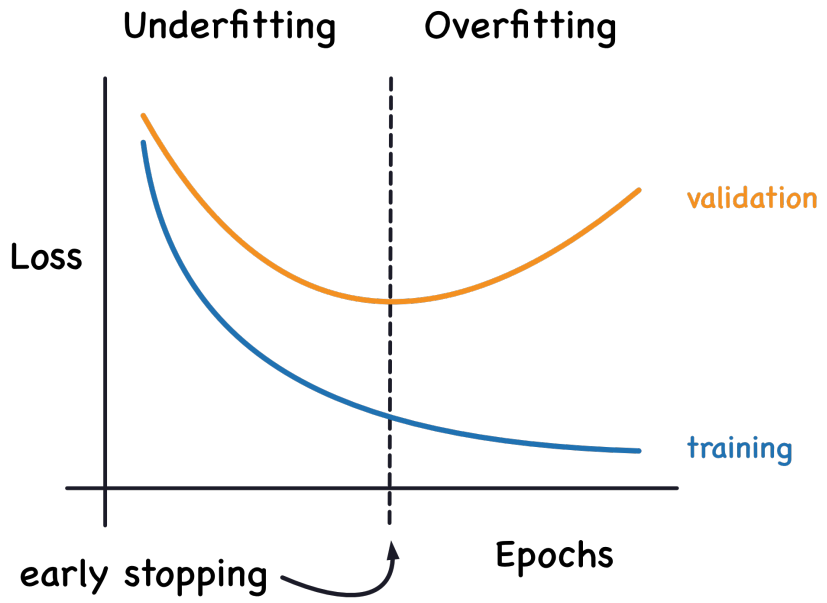
Training and test data

- We typically generate a few thousand simulations for training
- We reserve a proportion for testing emulator accuracy during training (early stopping)
- Prevents overfitting of the training data

```
# split the data
idx = random.sample(range(n), int(n*0.8))
train_params_pretile = parameters[idx]
train_signals_pretile = signals[idx]
test_params_pretile = np.delete(parameters, idx, axis=0)
test_signals_pretile = np.delete(signals, idx, axis=0)
```



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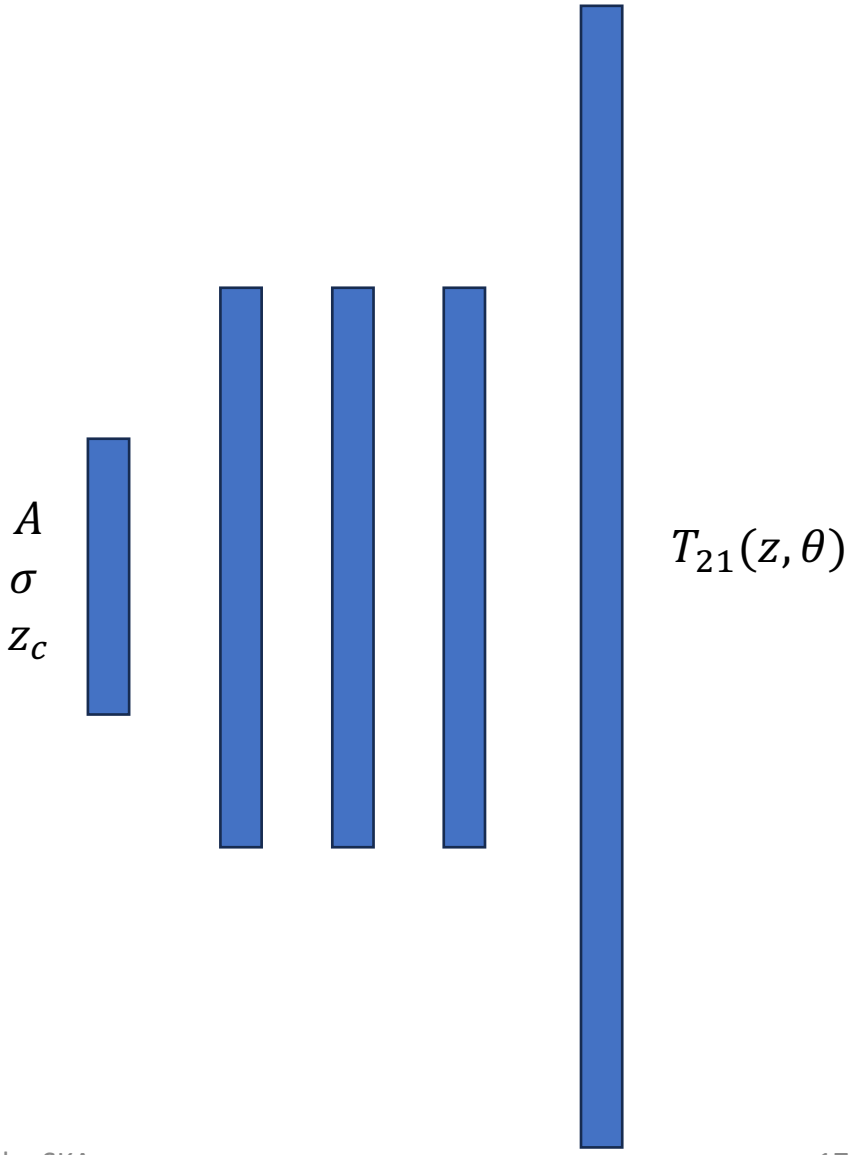
Architecture choices

- We could attempt to train a network to go directly from θ to $T_{21}(z)$
- However, we might want to evaluate the 21-cm signal at a range of different redshifts
- Leads to a big network and lots of parameters to optimize



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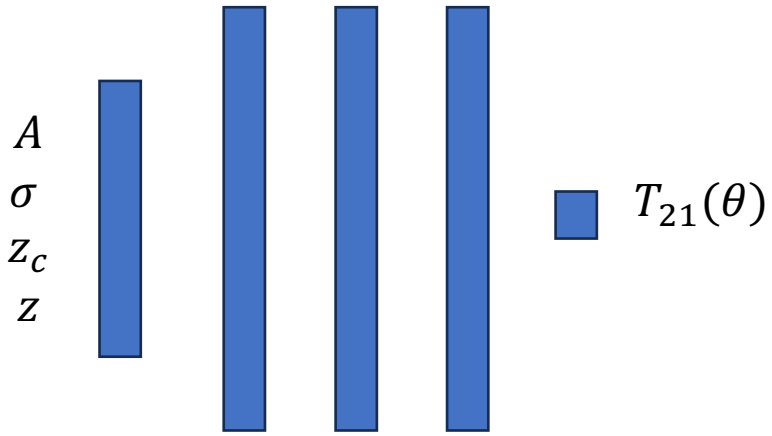
Architecture choices

- We could perform some form of dimensionality reduction such as PCA (see later)
- But for 21-cm Cosmology we choice to make redshift (the independent variable) an input to our network
- Loop over the network to predict $T_{21}(z, \theta)$



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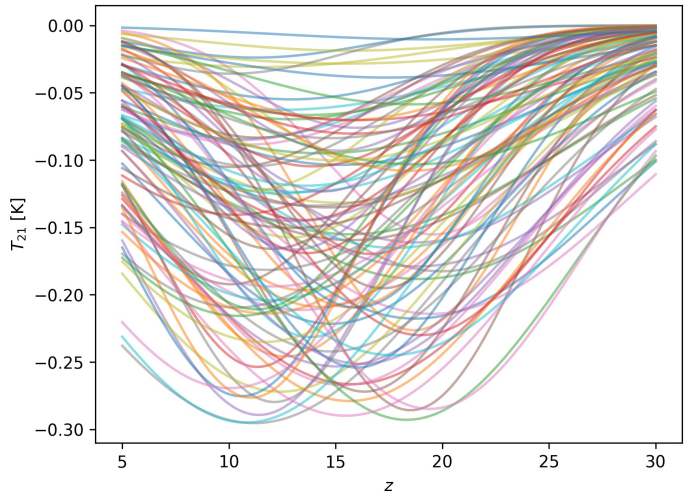
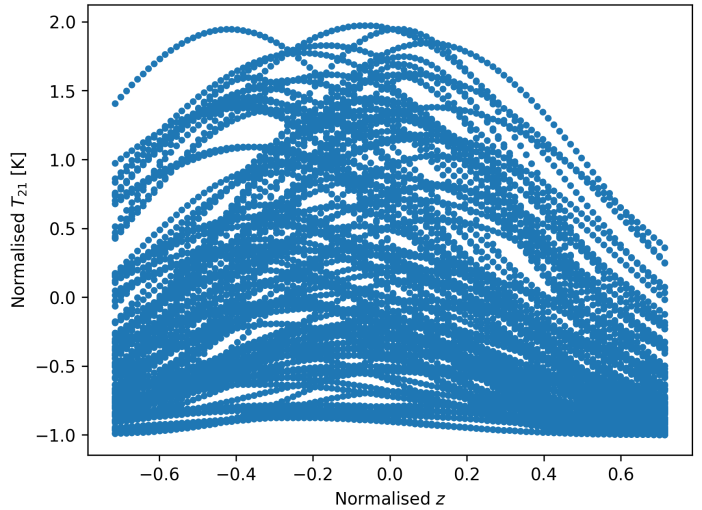
Normalisation and data processing

- We have to carefully format our data so that we input $\{A, \sigma, z_c, z\}$ and output $T_{21}(z, \theta)$

- Perform standardization on training and test data sets

$$\tilde{A} = \frac{A - \bar{A}}{\sigma_A}$$





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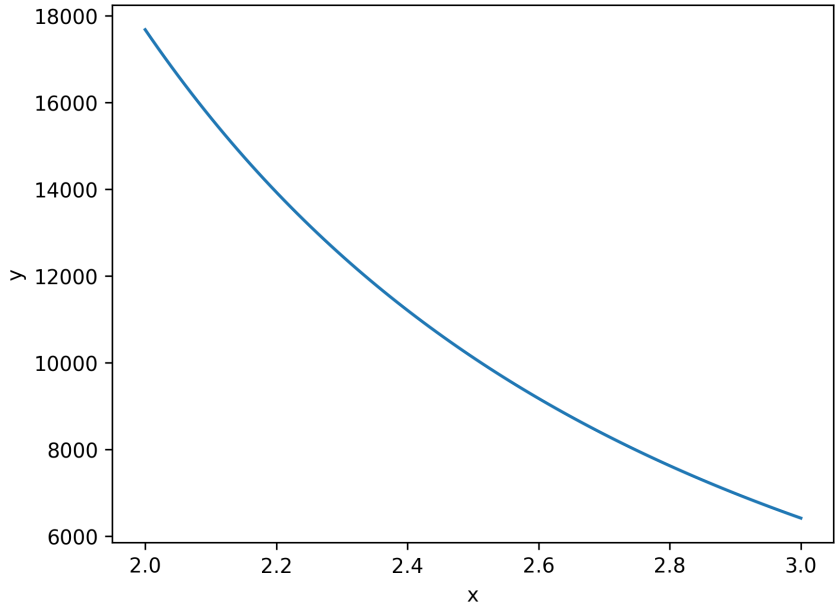
Why do we normalize?

- Imagine fitting a polynomial function to a power law data set

$$M = \sum_{i=0}^{N} a_i x^i$$

- If $x \sim 1, y \sim 10{,}000$ and $N = 3$ then the individual a_i can take on values between $-10{,}000$ to $10{,}000$



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Why do we normalize?

- But if we normalize so that y ~ 1 then our model is effectively

$$M = y_0 \sum_{i=0}^{N} a_i x^i$$

- And $a_i \sim 1$ making the problem much easier to fit

- By normalising we reduce the range of values that ϕ can take and make the problem easier to solve

- Activation functions are also usually set up to take in order unity values otherwise they saturate but this is by design i.e. not the reason we normalize

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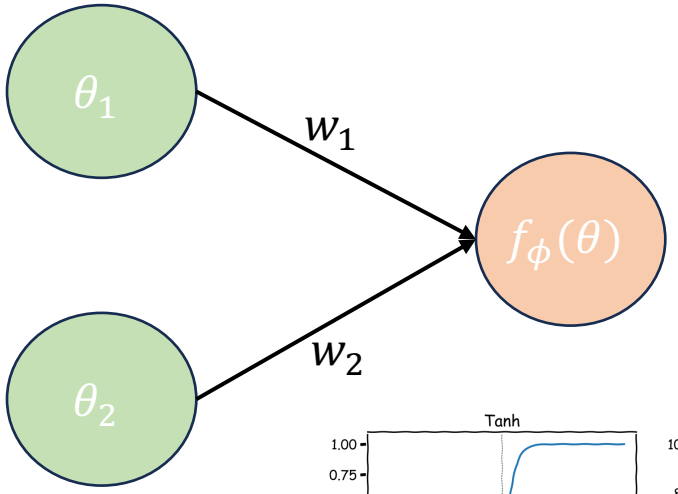
Activation Functions

- Activation functions add non-linearity into our modelling
- We often want to make careful choices for our activation functions
- E.g. if we know our output (after normalization) should be between 0-1 we might choose a sigmoid activation



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where

$$\phi = \{w_1, w_2\}$$

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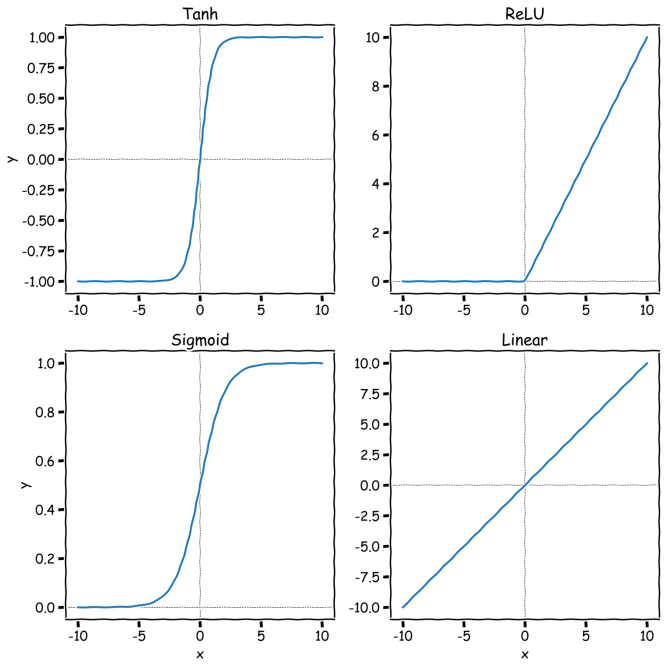

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Building the neural network

```
# callback for early stopping
callback = tf.keras.callbacks.EarlyStopping(monitor='val_loss', patience=10)

# neural network architecture
model = tf.keras.models.Sequential([
    tf.keras.layers.Dense(4, activation='sigmoid'),
    tf.keras.layers.Dense(8, activation='sigmoid'),
    tf.keras.layers.Dense(8, activation='sigmoid'),
    tf.keras.layers.Dense(8, activation='sigmoid'),
    tf.keras.layers.Dense(8, activation='sigmoid'),
    tf.keras.layers.Dense(1, activation='linear'),
])

# building the model with the adam optimizer and mean squared error loss function
model.compile(optimizer='adam',
              loss='mse',)
```

```
# training the model
model.fit(train_params, train_signals, epochs=200, batch_size=250,
          callbacks=[callback], validation_data=(test_params, test_signals))
```

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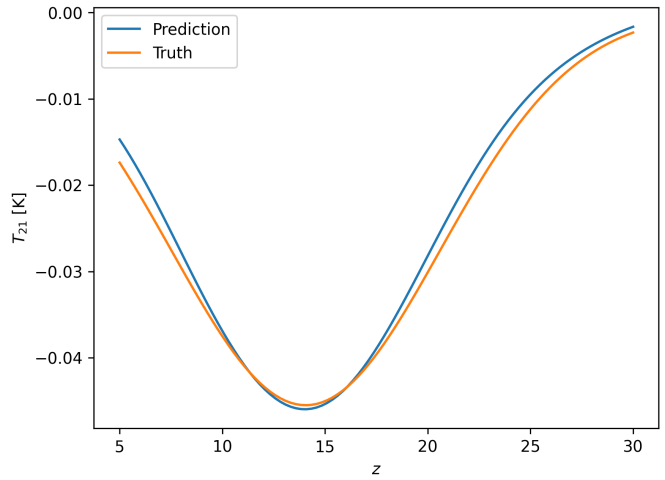
Assessing the accuracy

- Once trained we want to assess whether the network is doing a good job before we use it in our Bayesian analysis

- The network will predict signals in the normalized space

```
def prediction(params):
    """
    This function takes in a set of unormalized parameters (A, zc, sigma)
    and returns a predicted signal in the unormalized space.
    """
    params = np.tile(params, len(z)).reshape(len(z), 3)
    params = np.hstack((params, z.reshape(-1, 1)))
    params = (params - norm_param_means) / norm_param_stds
    pred = model.predict(params, verbose=0)
    return pred*norm_signal_stds + norm_signal_means

pred = prediction(test_params_pretile[100])
plt.plot(z, pred)
plt.plot(z, test_signals_pretile[100])
plt.xlabel('z')
plt.ylabel('signal')
plt.show()
```



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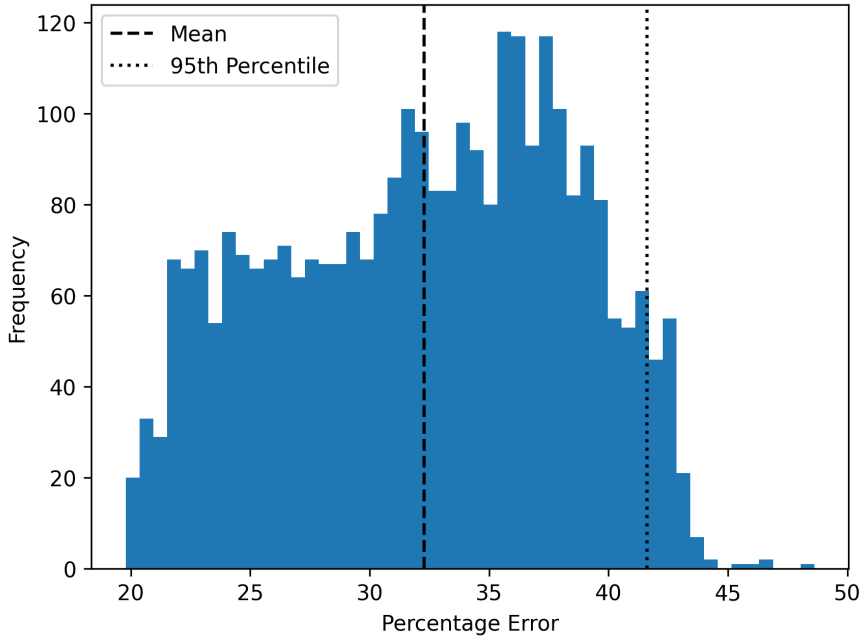
Assessing the accuracy

- Often we want a more general measure of accuracy
- We assess on the whole test data set and take the average and 95th percentile values
- This network isn't very accurate!

```
error = []
for i in tqdm(range(len(test_params_pretile))):
    pred = prediction(test_params_pretile[i])
    error.append(100*np.mean(np.abs(pred - test_signals_pretile[i]))
                 /np.max(np.abs(test_signals_pretile[i])))
error = np.array(error)
```



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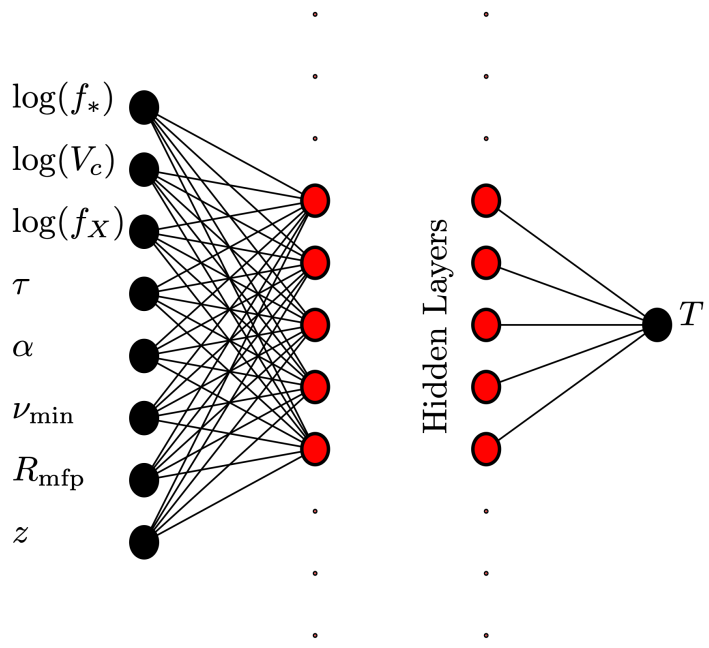
Current state of the art

- There are many approaches for emulating the sky-averaged 21-cm signal
- globalemu uses some of the ideas discussed here
- It is light weight, easy to retrain and very fast while maintaining a good level of accuracy
- https://arxiv.org/abs/2104.04336

globalemu: Robust and Fast Global 21-cm Signal Emulation

Introduction

globalemu:	Robust Global 21-cm Signal Emulation
Author:	Harry Thomas Jones Bevins
Version:	1.8.2
Homepage:	https://github.com/htjb/globalemu
Documentation:	https://globalemu.readthedocs.io/



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Current state of the art

- 21cmVAE uses Variational Autoencoders
- More complicated architecture, harder to retrain and an order of magnitude slower than globalemu
- But more accurate than globalemu
- https://arxiv.org/abs/2107.05581

21cmVAE: A Very Accurate Emulator of the 21-cm Global Signal

Christian H. Bye,[1,2] Stephen K. N. Portillo,[3] and Anastasia Fialkov[4,5]

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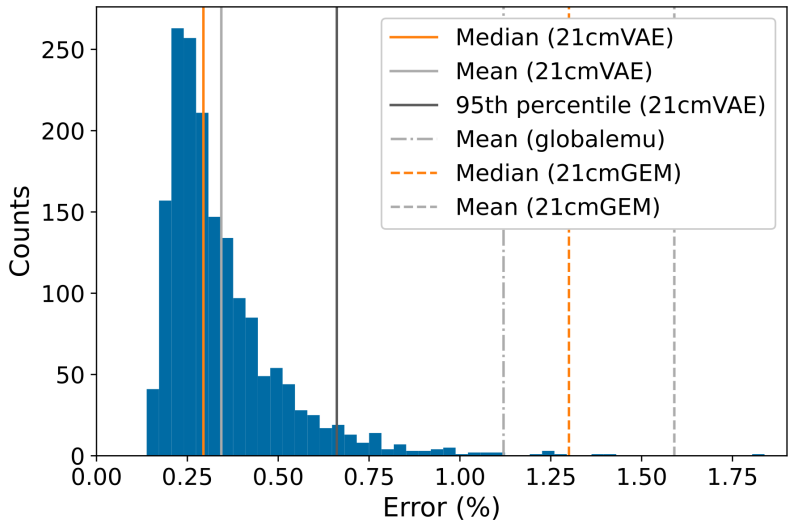
Submitted to ApJ

ABSTRACT

Considerable observational efforts are being dedicated to measuring the sky-averaged (global) 21-cm signal of neutral hydrogen from Cosmic Dawn and the Epoch of Reionization. Deriving observational constraints on the astrophysics of this era requires modeling tools that can quickly and accurately



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Dimensionality Reduction

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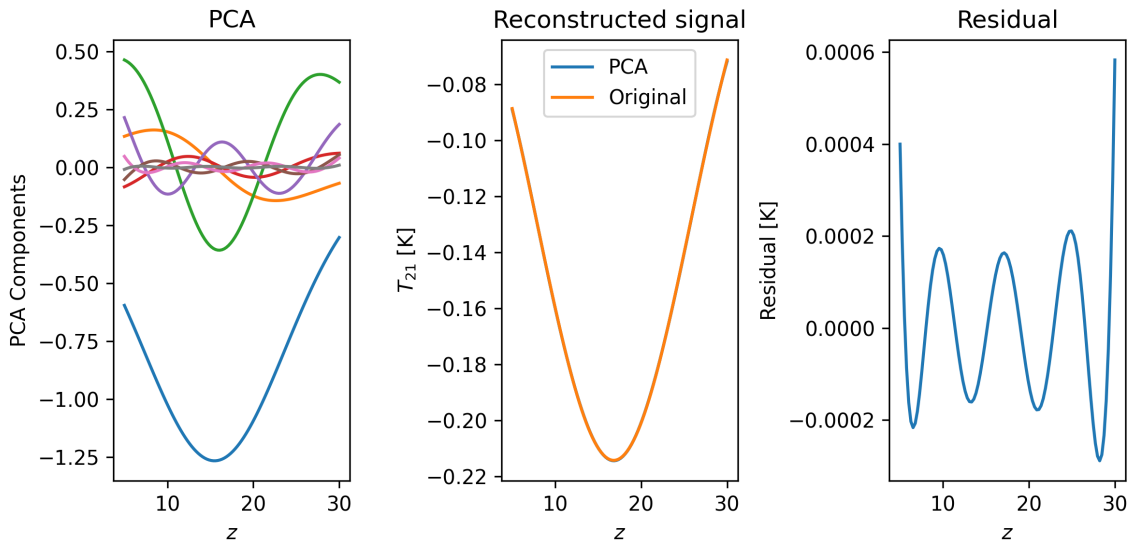
Principle Component Analysis

- Dimensionality reduction technique
- Decompose training data into eigenvectors and order based on eigenvalues
- Eigenvectors with largest eigenvalues describe the directions in the training data with the biggest variance
- Discard eigenvectors that correspond to low variance directions
- Reconstruct signals with weighted sum of most important eigenvectors where weights vary for each signal



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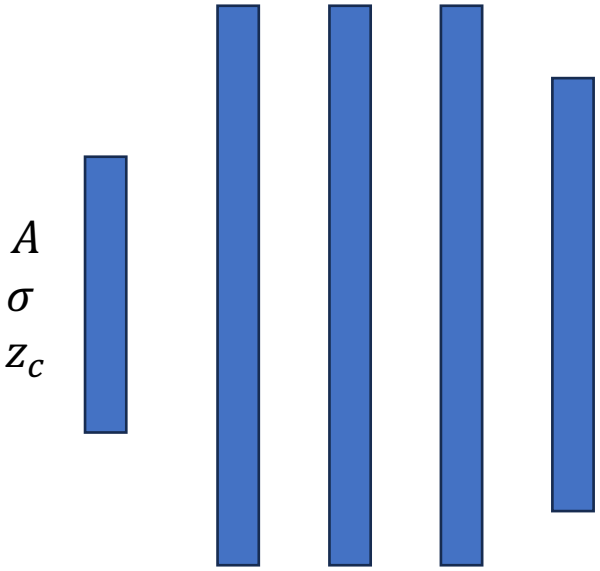
Principle Component Analysis



A
σ
z_c

Signal Specific PCA coefficients $\times$ Important eigenvectors $\longrightarrow$ Sum terms $= T_{21}\,(z, \theta)$

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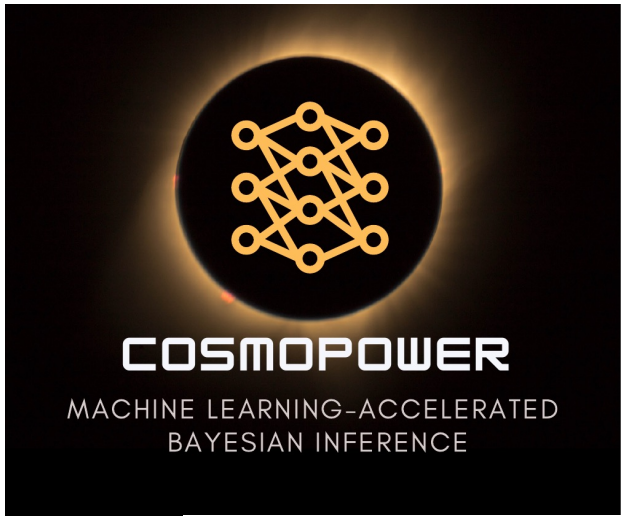
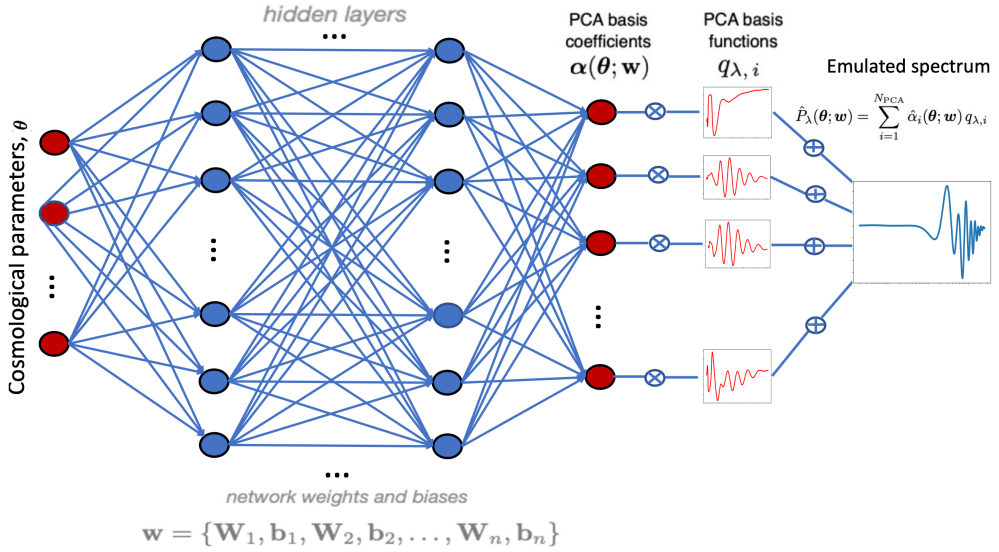
Cosmopower



- Emulating the CMB power spectrum as a function of cosmological parameters
- Very accurate and easily retrainable
- Uses Principle Component Analysis
- https://arxiv.org/abs/2106.03846



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21-cm 2D Power Spectrum with the SKA

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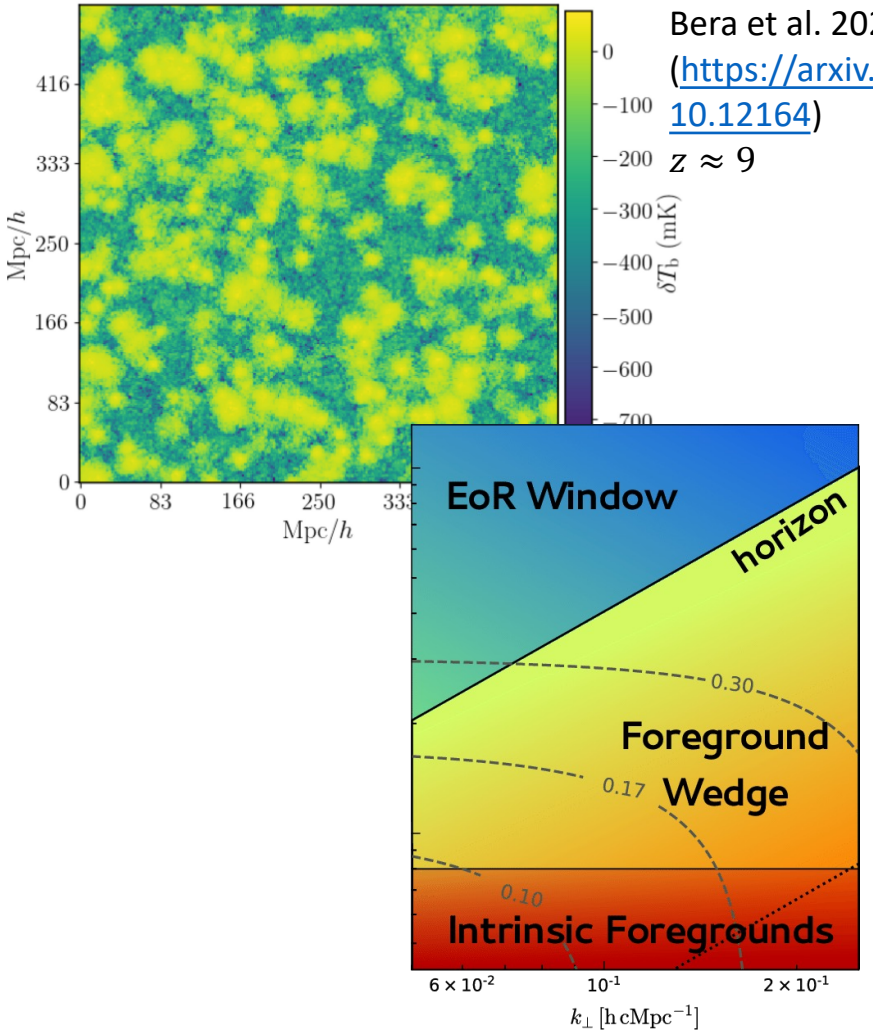
The SKA and 21-cm Cosmology

- The SKA will attempt to measure how the 21-cm signal varies spatially and temporally on the sky

- And extract science via the 2D power spectrum



Bera et al. 2022 (https://arxiv.org/abs/2210.12164)
$z \approx 9$

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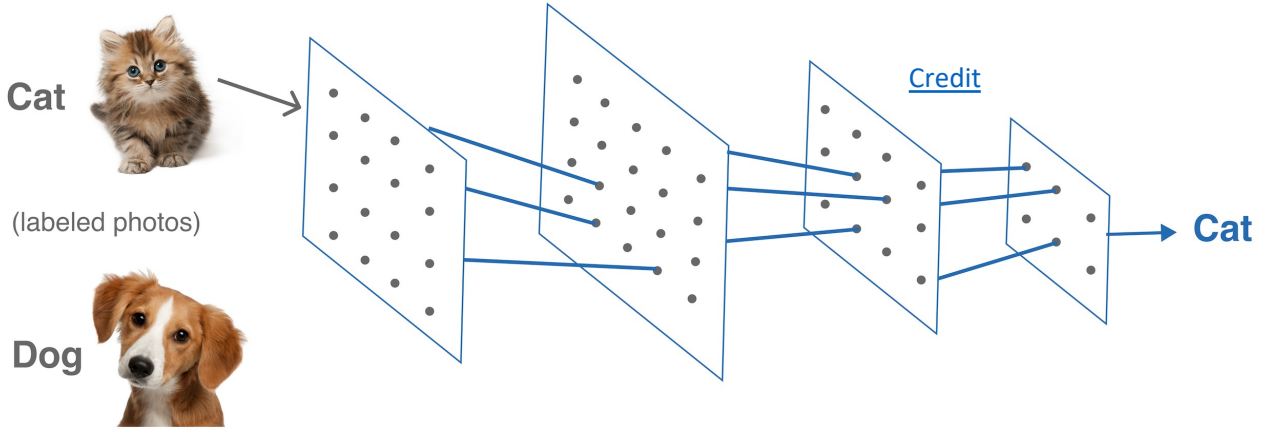
How do we emulate images?

- One way to emulate 2D images is with Convolutional Neural Networks
- Traditionally used for pattern recognition
- And subsequent classification of images



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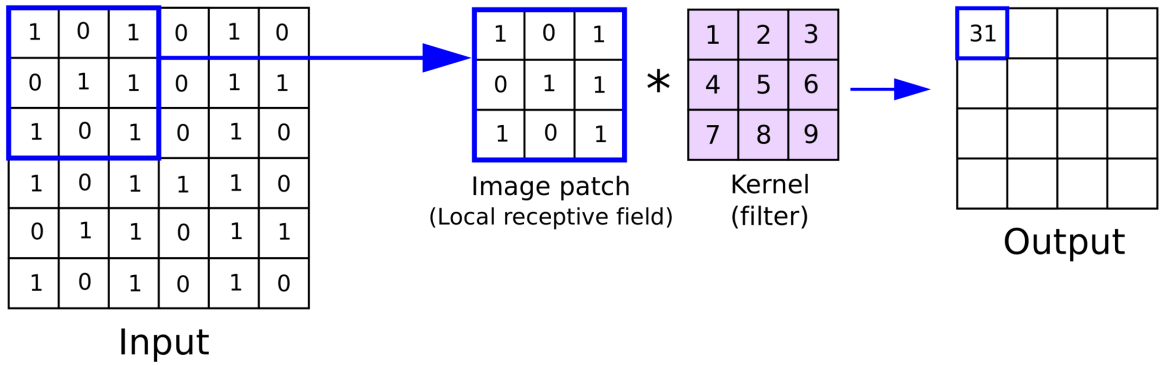
Convolutional Layers

- Convolutional layers take an image and slide a filter across the image performing a dot product as they go
- Many filters are used to pick out key features gives you a stack of filtered images or a volume
- Filters can be 2D or 3D in nature to increase or decrease the volume of the feature space at each layer



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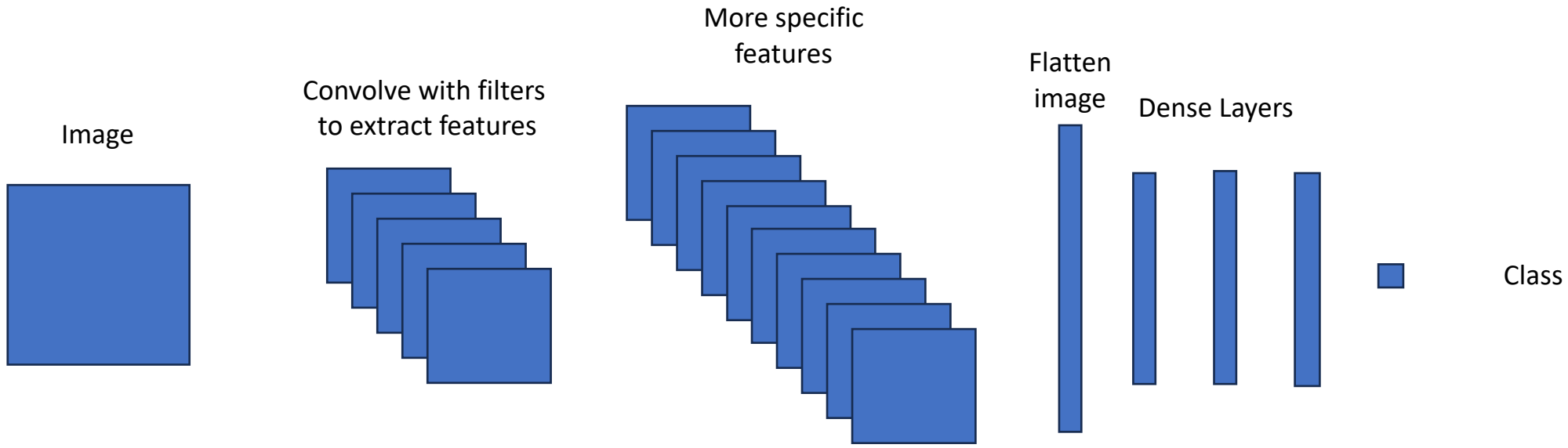
Convolutional Neural Networks



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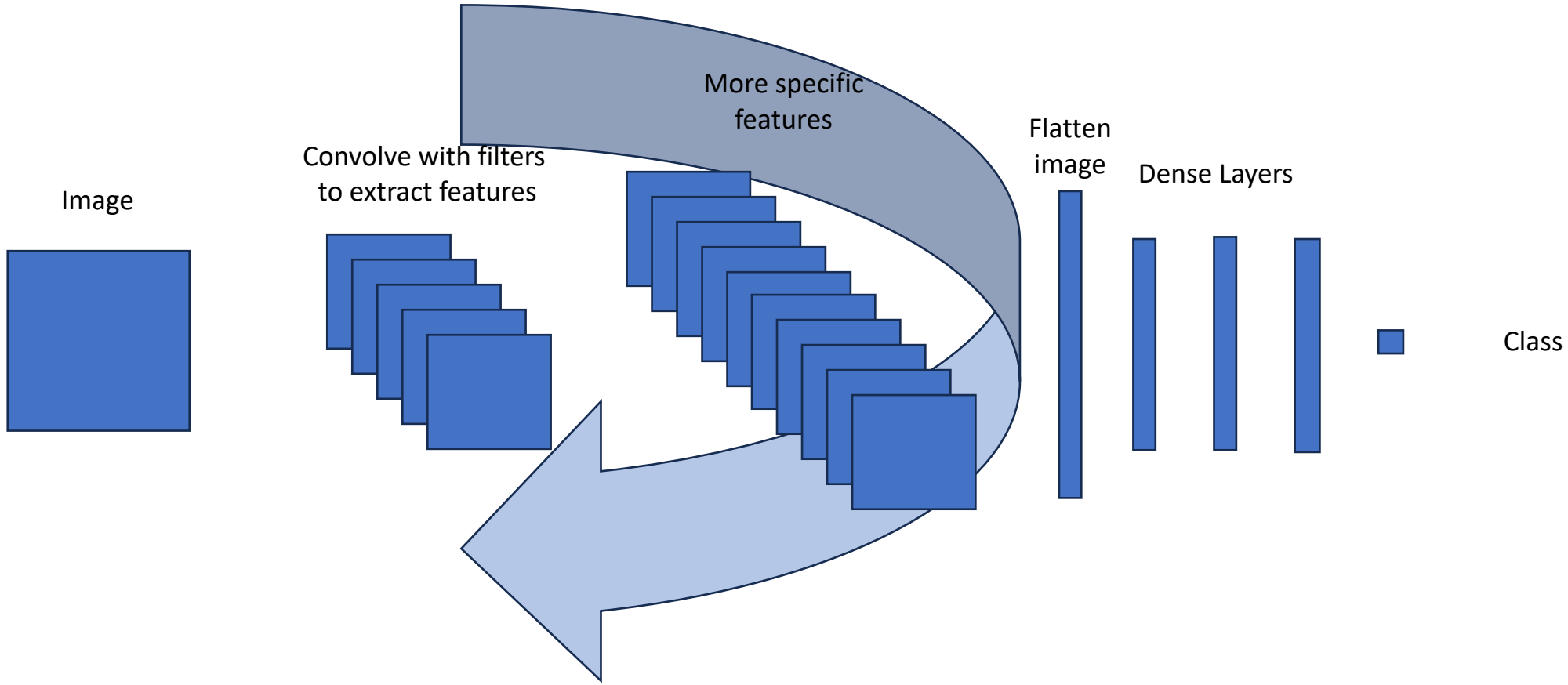
As Emulators



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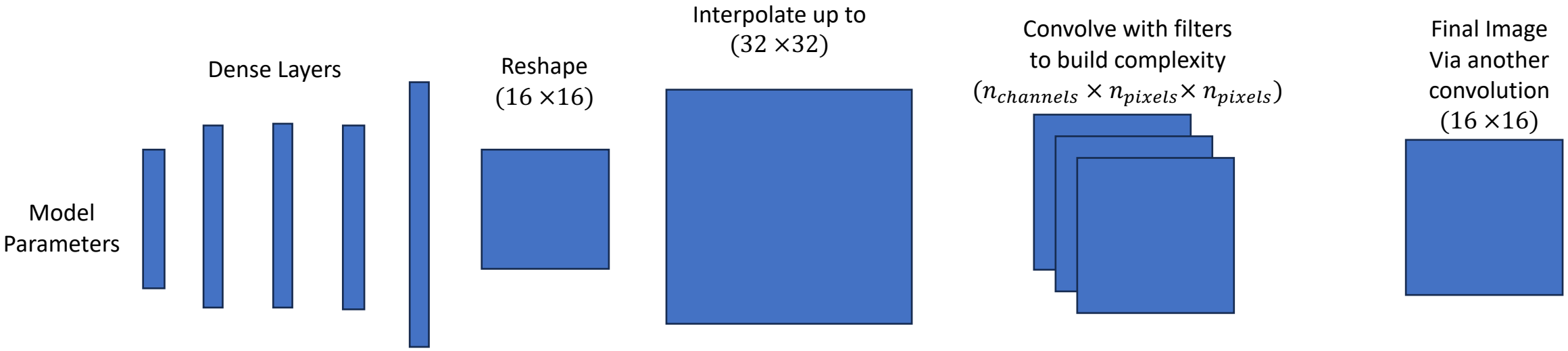
As Emulators



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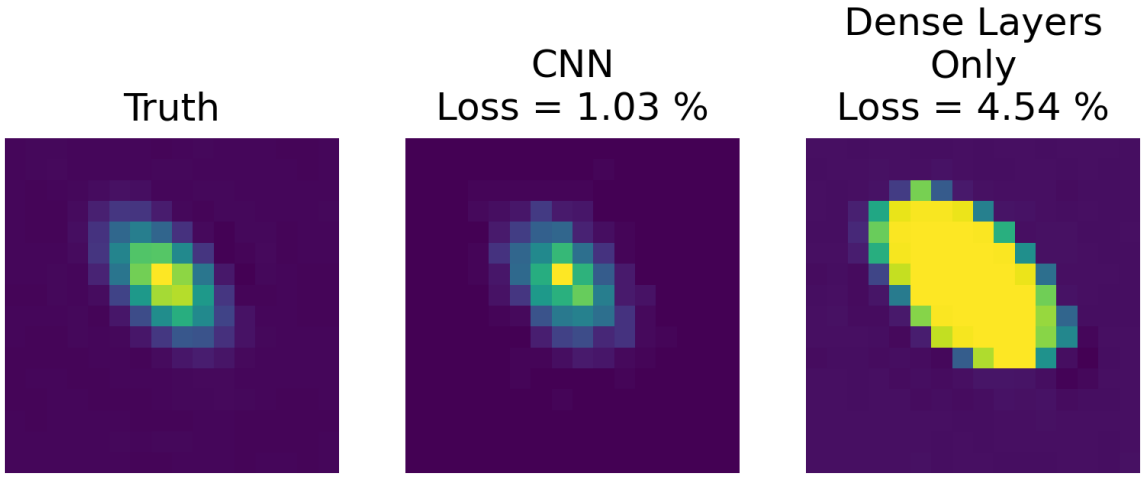
An Example

- Multivariate 2D Gaussian with random covariance and means
- Histogram in (16 x 16) grid where each bin represents a pixel with some intensity
- Train a network with Convolutional layers and interpolation and a network with just dense layers for comparison



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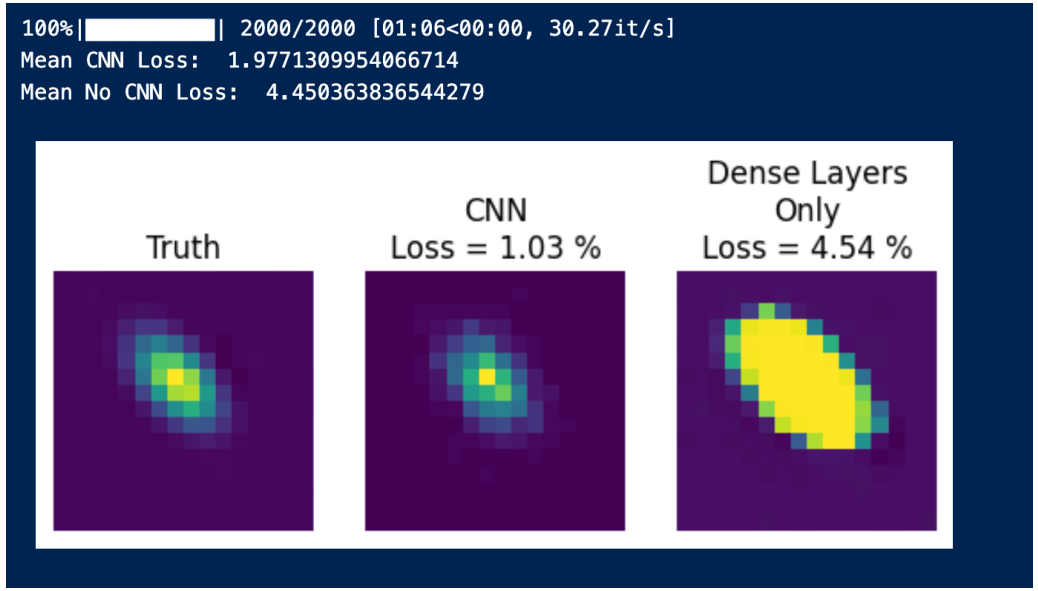
Optimisation

- The values of the filters are optimized in the same way as the weights in a fully connected network to minimize ϵ_ϕ

- Define a pixel by pixel loss between the image and the prediction



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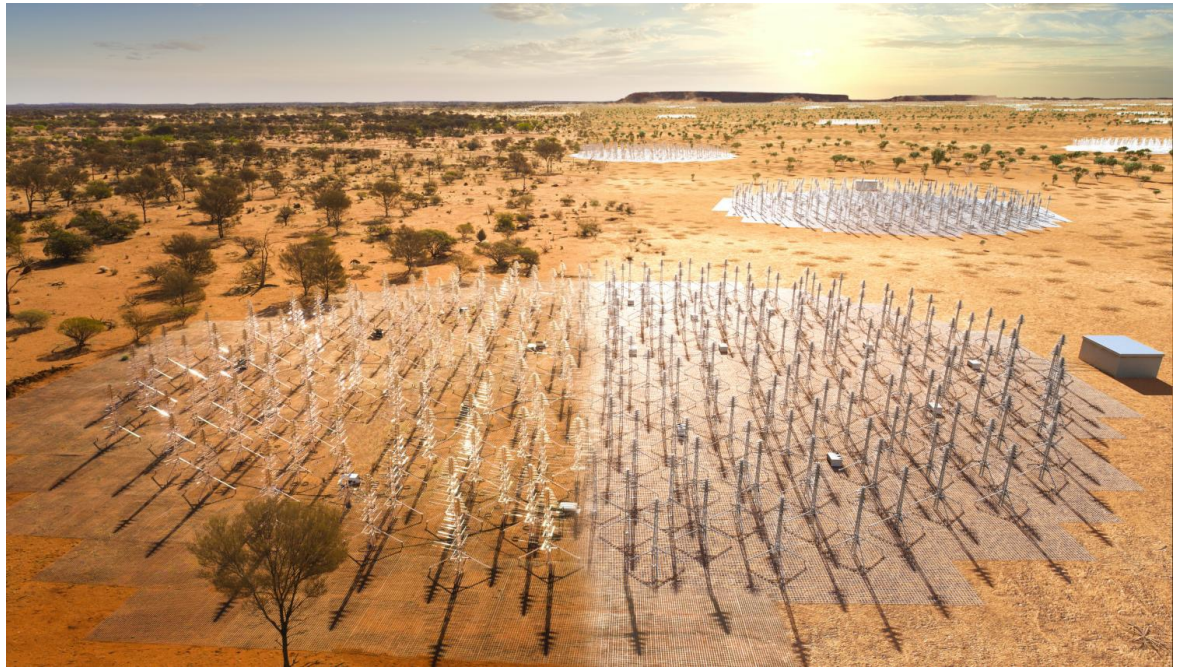
For the SKA 21-cm Observations

- The likelihood is going to be on the power spectrum
- Emulator takes us from astrophysics to the 2D power spectrum
- An example application using CNNs to directly emulate the 2D power spectrum can be found in 21cmEMU (https://arxiv.org/abs/2309.05697)



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Summary

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Emulators allow us to do inference

- Emulators are an efficient way to approximate complex semi-numerical simulations
- They take of order milliseconds to evaluate compared to hours per realization making inference possible
- Sensible choices about architectures, use of dimensionality reduction techniques, activation functions, loss funcitons etc can make a big difference to the run time and accuracy of emualtors

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Many different ways to do this

- Host of different tools that can be used to build emulators
  - Here we have looked at Dense Neural Networks and Convolutional Neural Networks
  - But we can also do this with Normalizing Flows and Gaussian Processes for example

Slides available at https://github.com/htjb/Talks (and Moodle!)
Example codes on github too!

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Next Lecture: Simulation Based Inference

- Why not just emulate the whole likelihood?