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Lecture 15
Signal Emulation for Astrophysics and Cosmology

Lecturer: **Dr Harry Bevins** (htjb2)

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

Posterior: P(θ)

Evidence: Z

Likelihood: $L(\theta)$

Prior: $\pi(\theta)$

$$\underbrace{P(\theta|D)P(D)}_{\text{Outputs}} = \underbrace{P(D|\theta)P(\theta)}_{\text{Inputs}}$$

For MCMC or Nested Sampling

The likelihood function

- The likelihood function gives the probability of the *data given the model and parameters* $L(\theta) = P(\theta|D, M)$
- 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

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

- 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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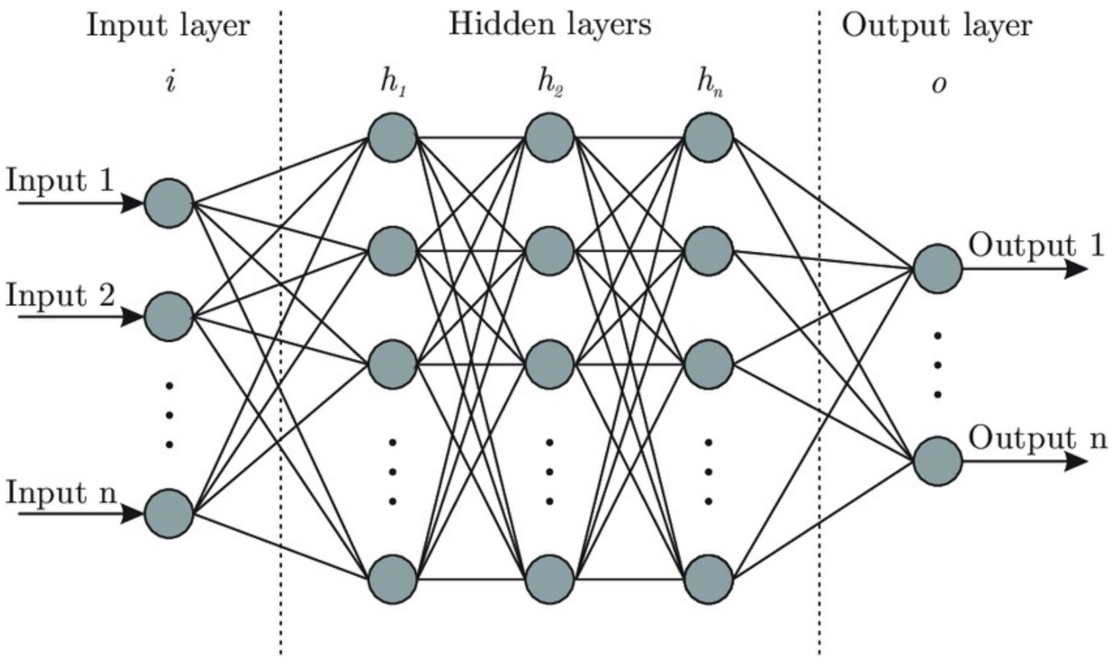
The issue

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

- 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

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



Sky-averaged 21-cm Cosmology

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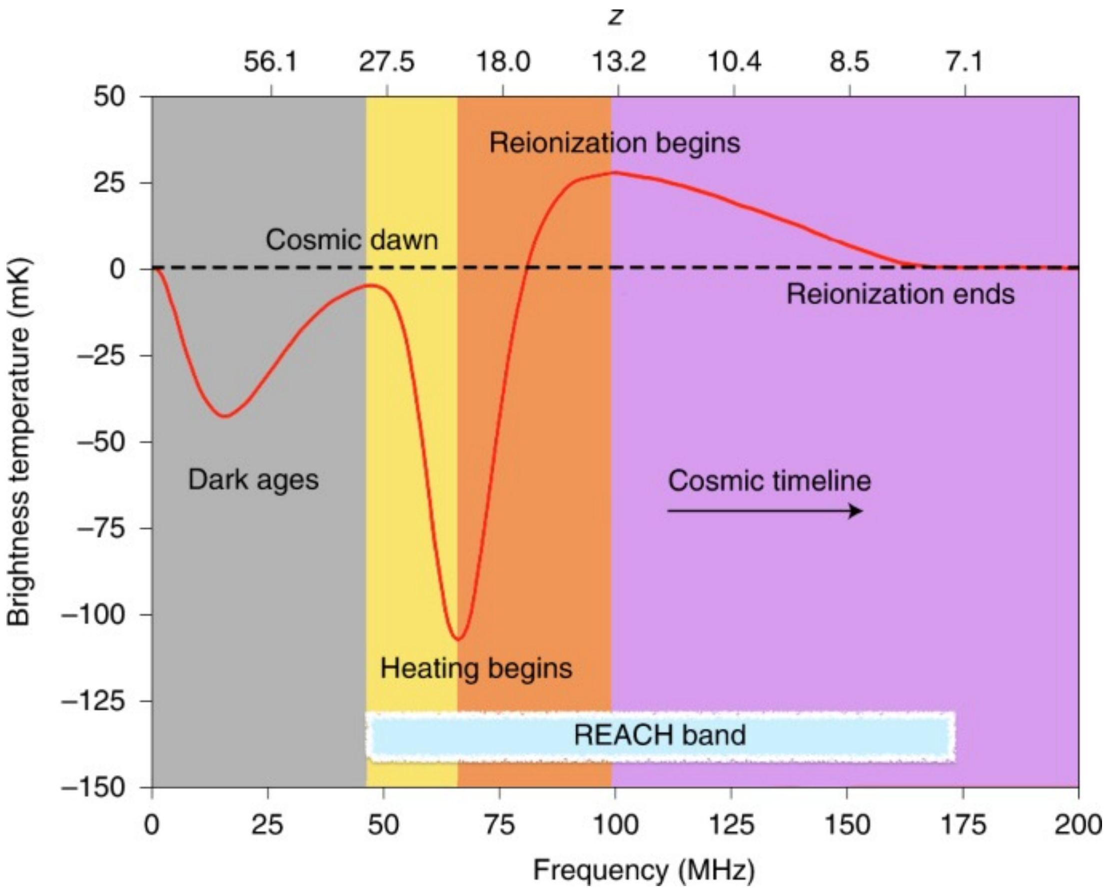
Sky averaged 21-cm Cosmology

- 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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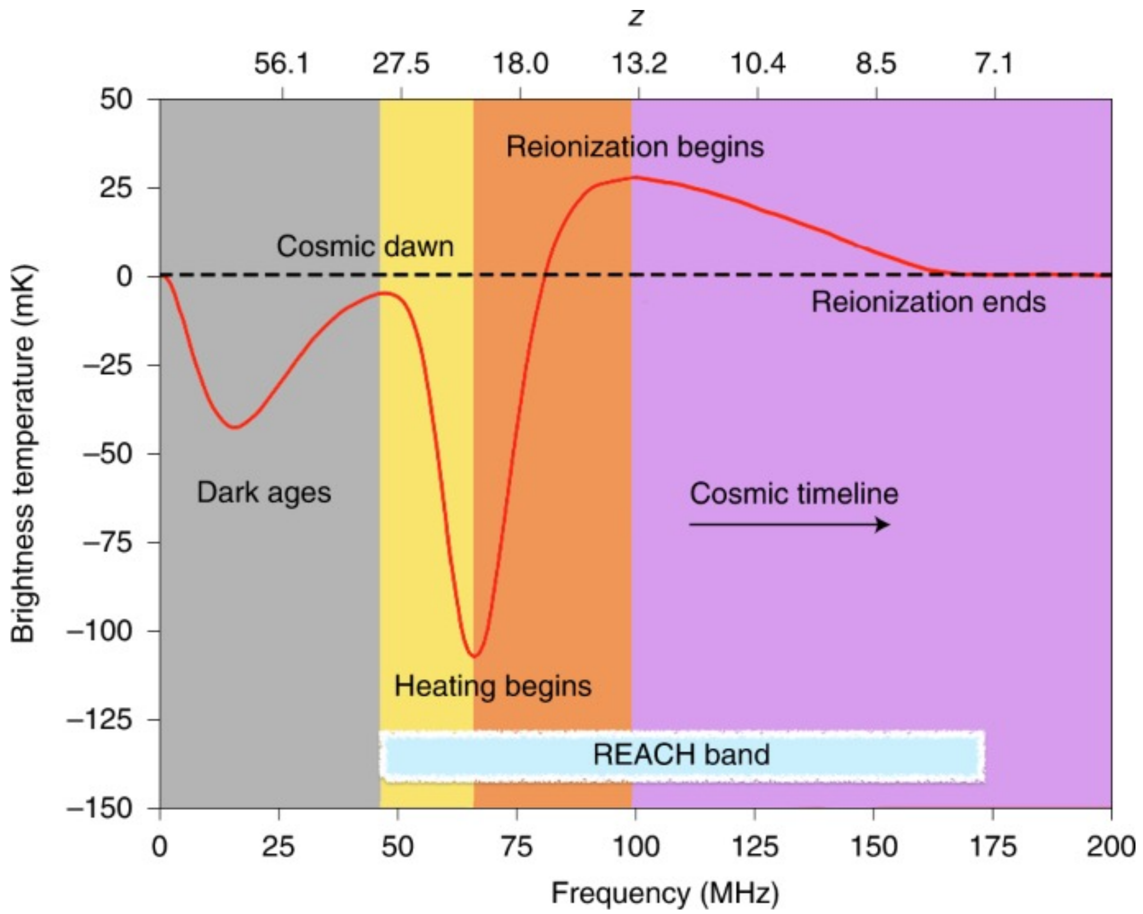
Sky averaged 21-cm Cosmology

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



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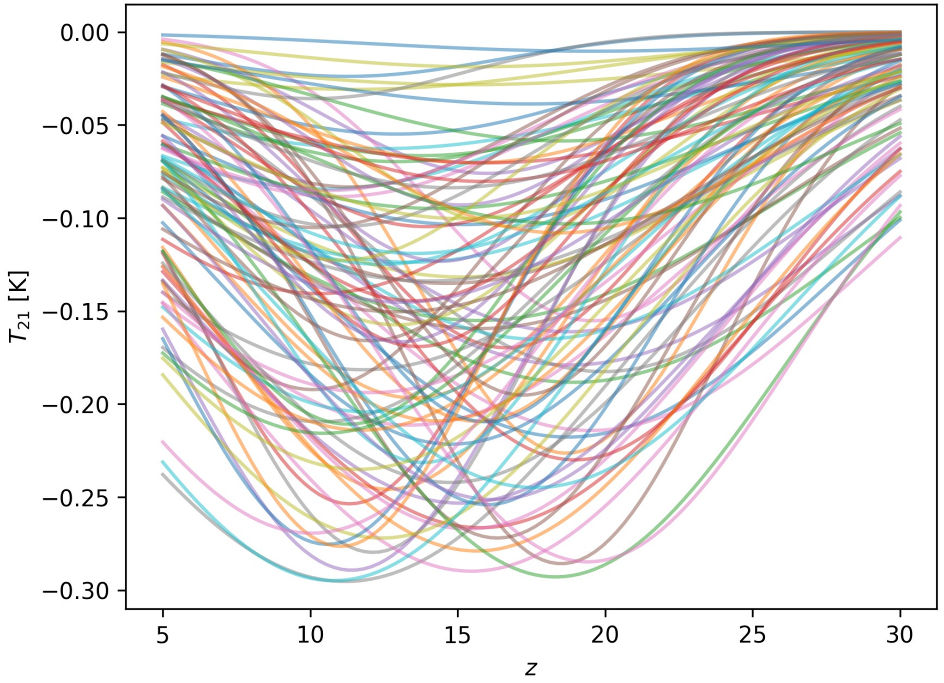
A toy 21-cm Cosmology example

- 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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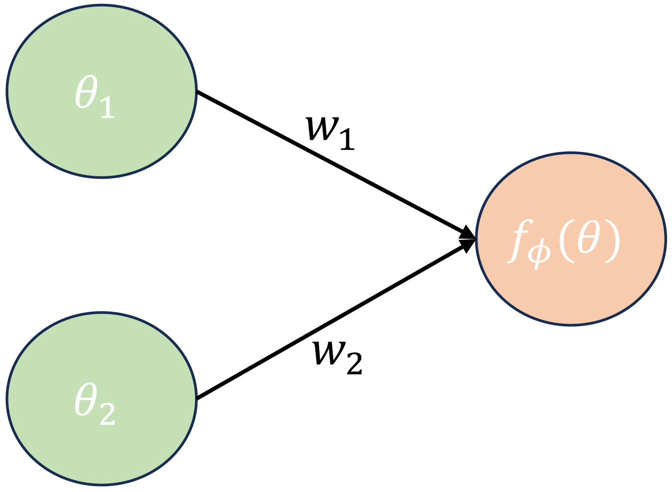
Emulators as an approximation

- 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

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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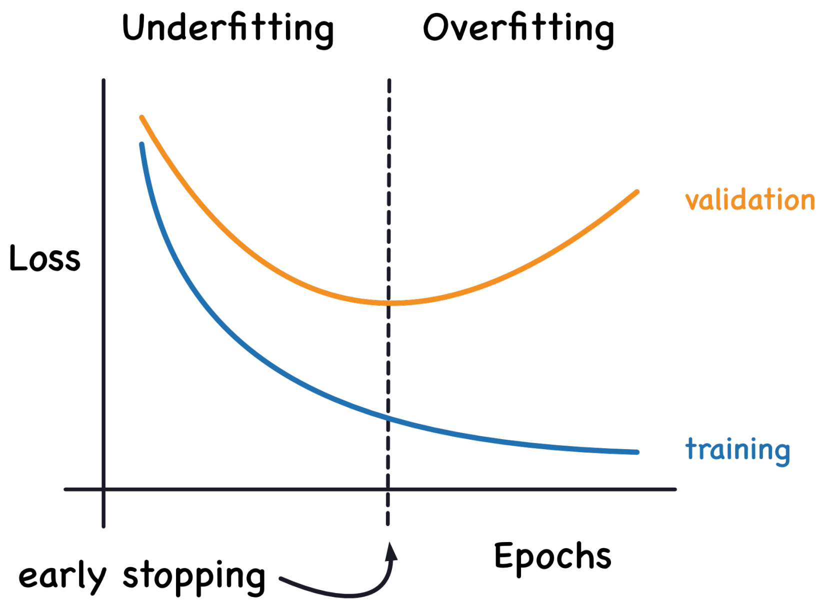
Training and test data

- We typically generate a few thousand simulations for training

```
# 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)
```

- We reserve a proportion for testing emulator accuracy during training (early stopping)



- Prevents overfitting of the training data

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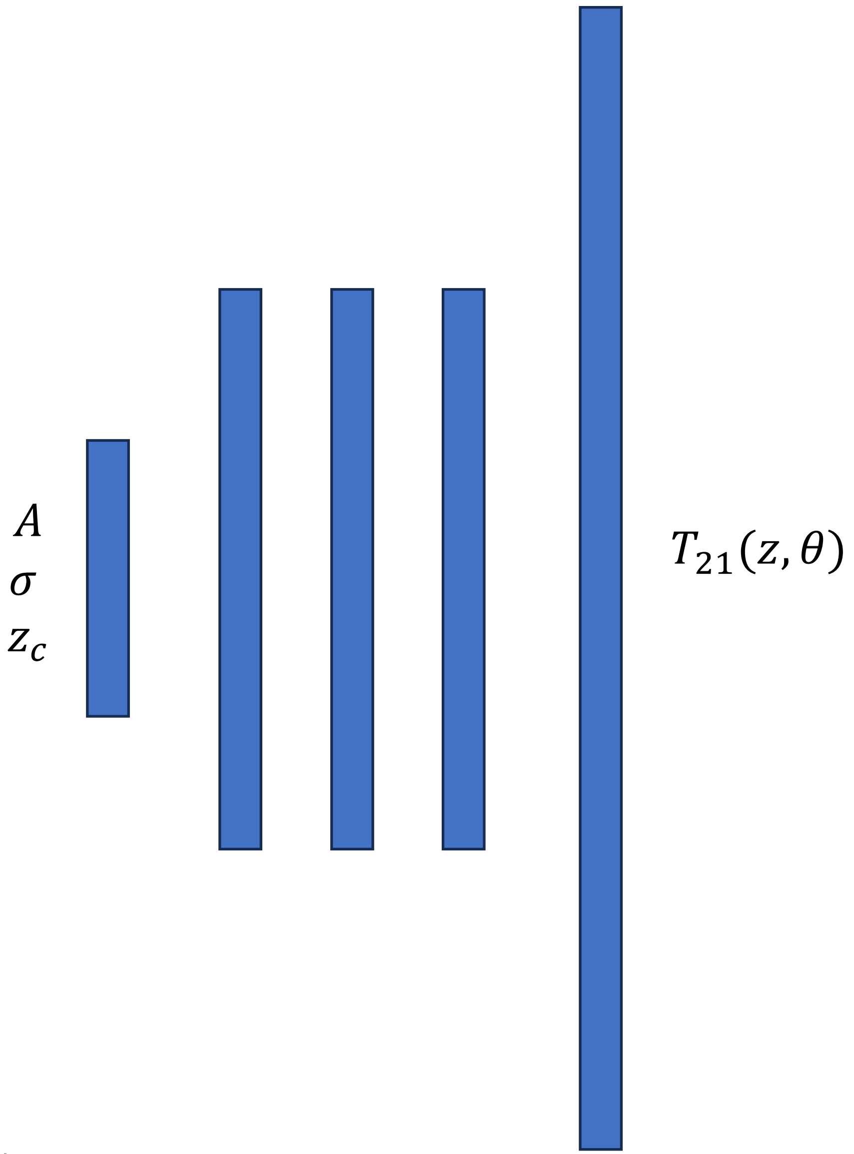
Architecture choices

- 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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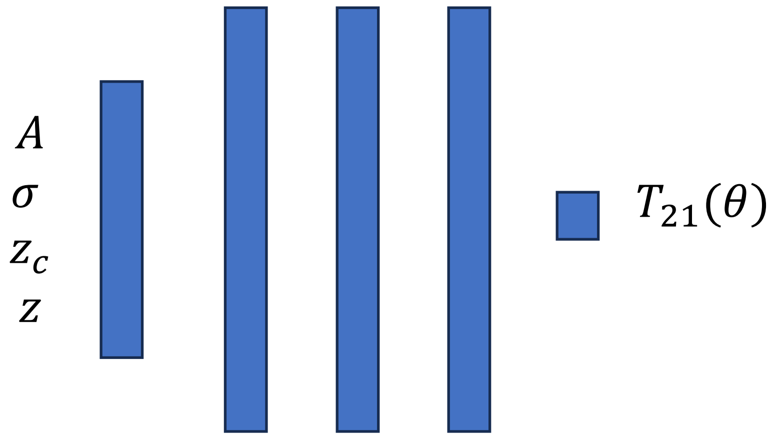
Architecture choices

- 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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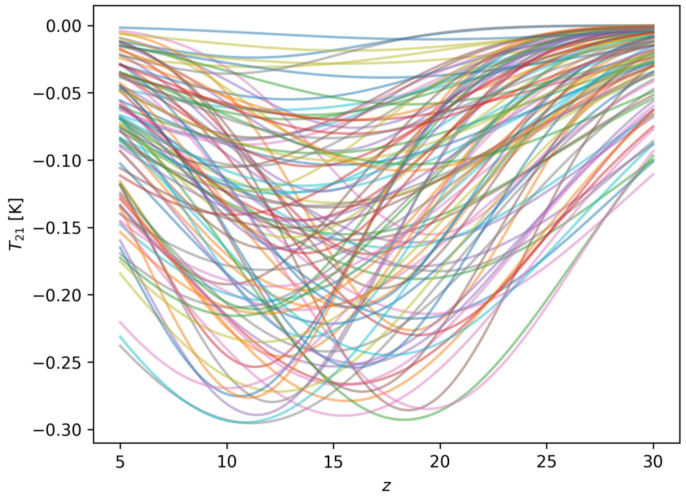
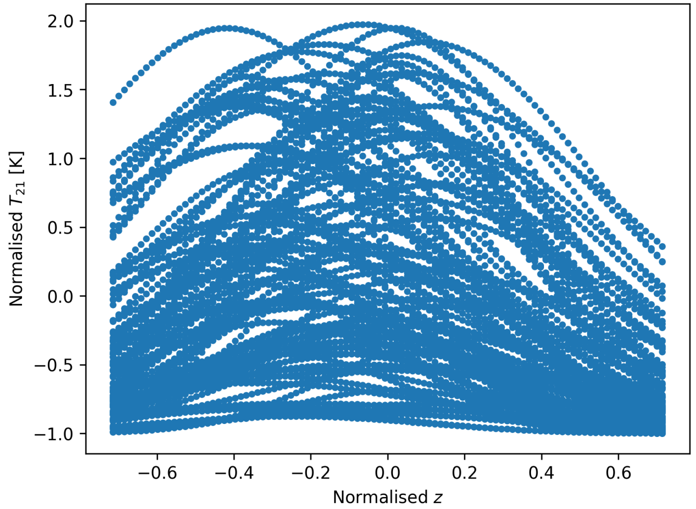
Normalisation and data processing

- Have to tile our training and test data (see the python notebook)

- Then standardize the inputs and outputs to the network using the mean and standard deviation of training data





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Why do we normalize?

- Imagine fitting a polynomial function to a power law structure

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

- If $x \sim 1$ and $y \sim 10{,}000$ then 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?

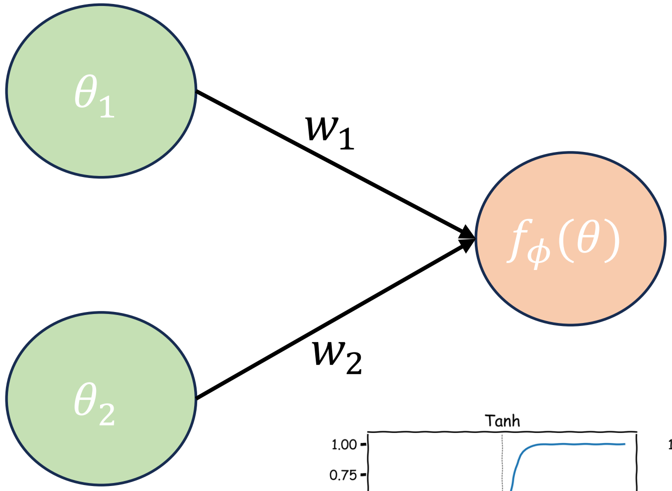
- But if we normalize so that y ~ 1 then our model is effectively

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

- And $a_i \sim 1$ making the problem much easier to fit
- For neural networks the idea is essentially to 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

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



$$f_\phi(\theta) = \sigma(w_1\theta_1 + w_2\theta_2)$$
where
$$\phi = \{w_1, w_2\}$$
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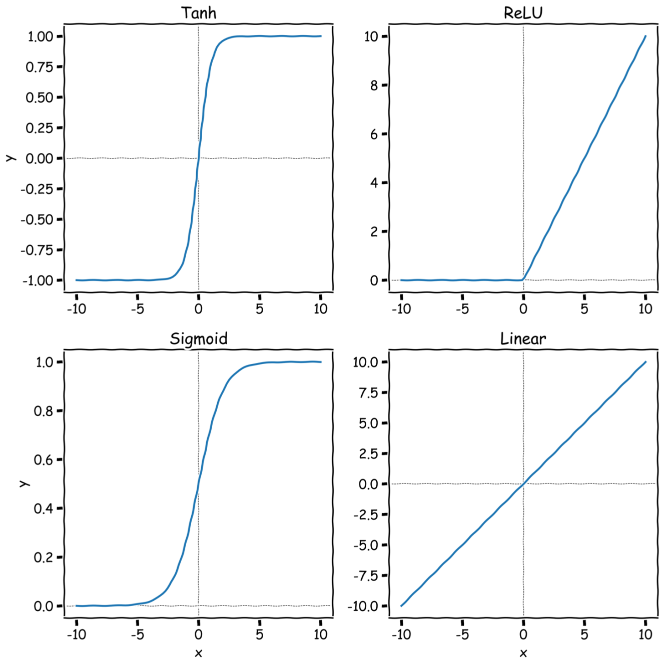

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Building the neural network

```
# 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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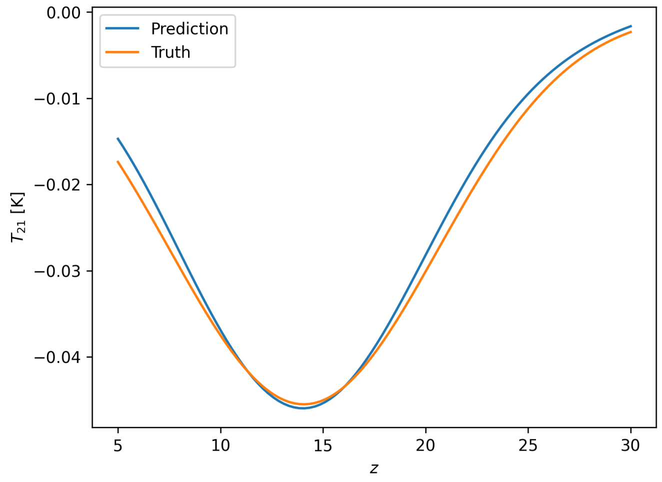
Assessing the accuracy

- 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

```python
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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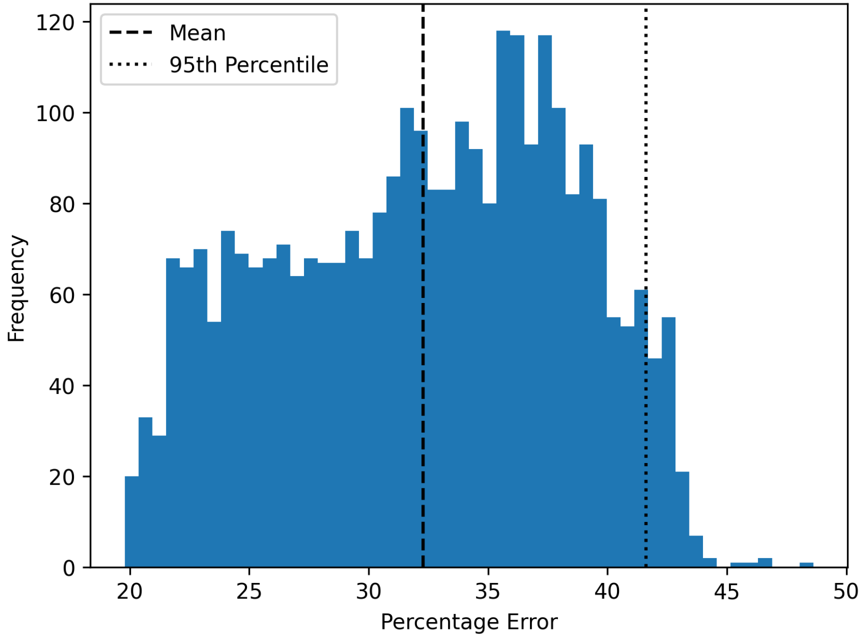
Assessing the accuracy

- Often we want a more general measure of accuracy
- We assess on the whole training 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)
```



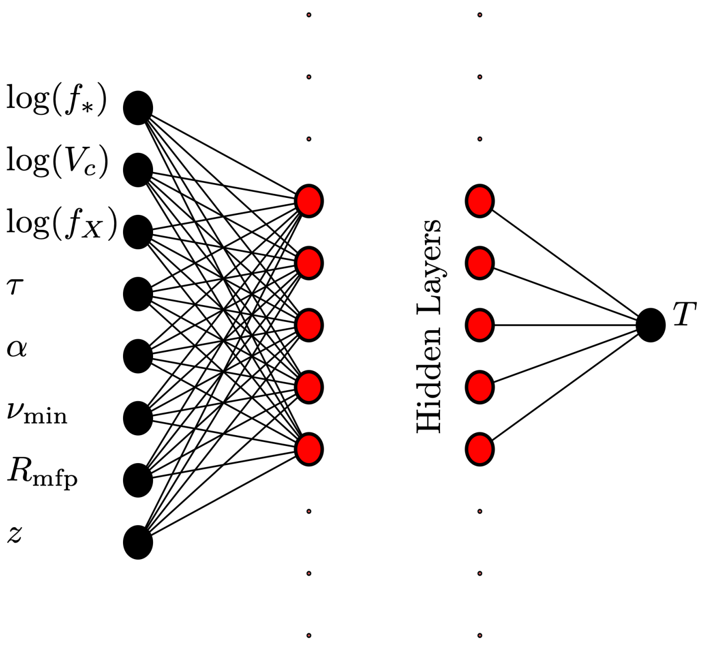
Current state of the art

- 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

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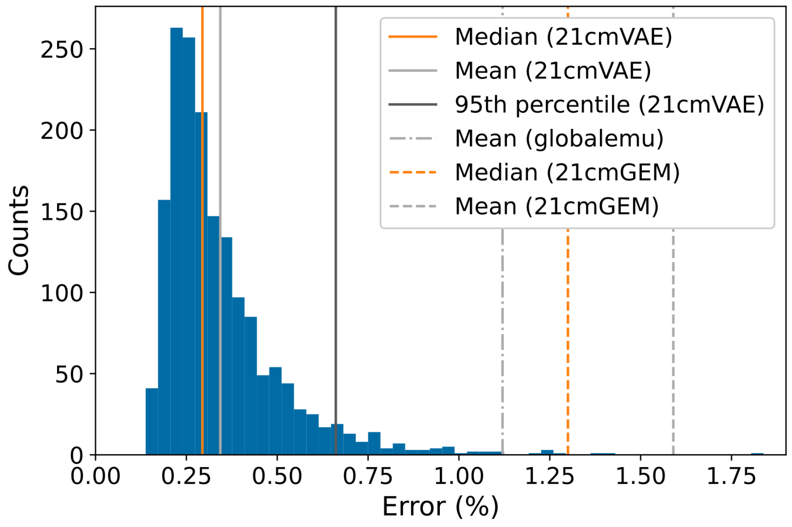
Submitted to ApJ

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



Dimensionality Reduction

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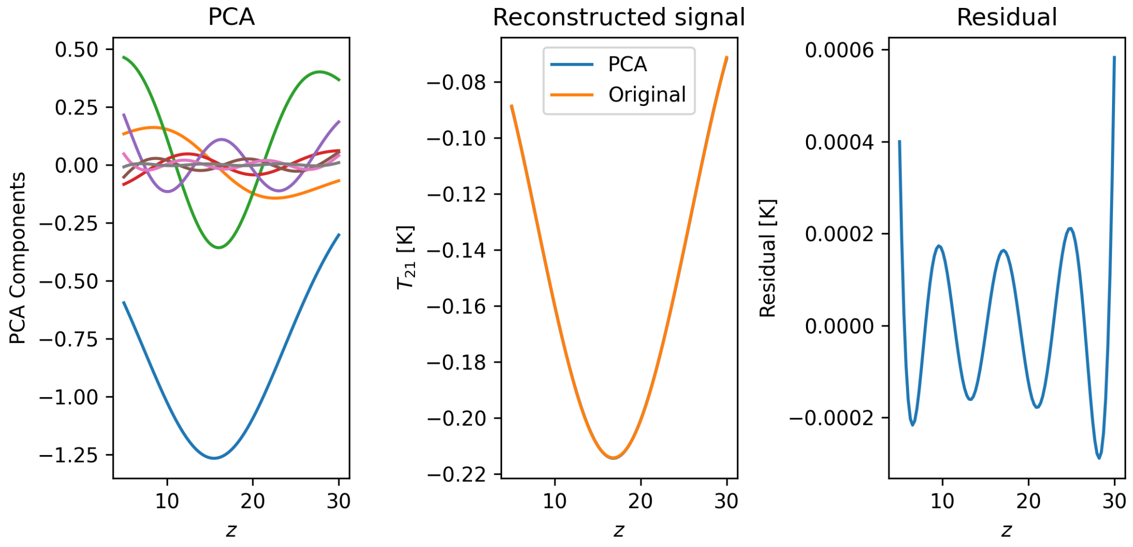
Principle Component Analysis

- 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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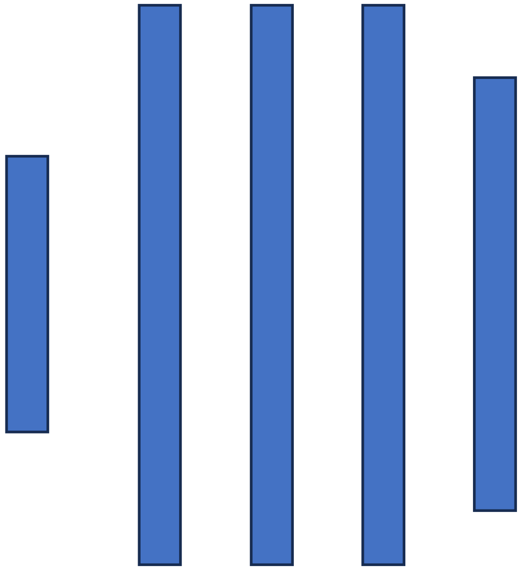
Principle Component Analysis

A
σ
z_c



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

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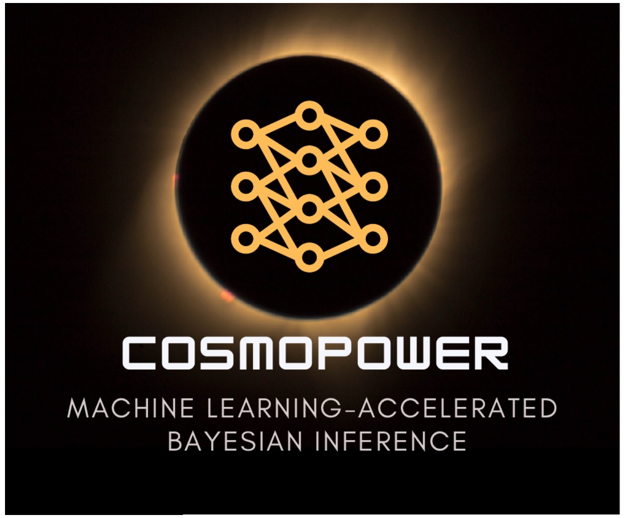
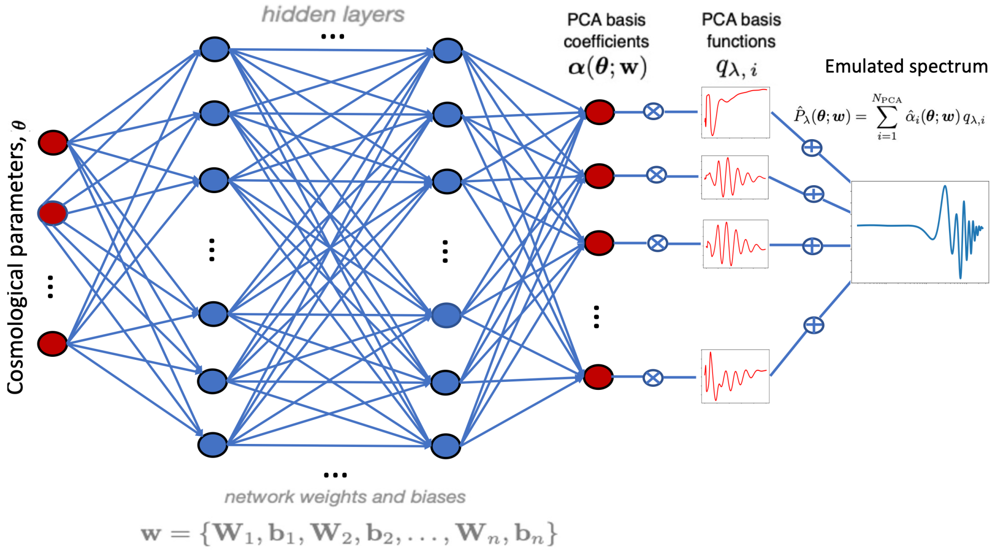
Cosmopower



- 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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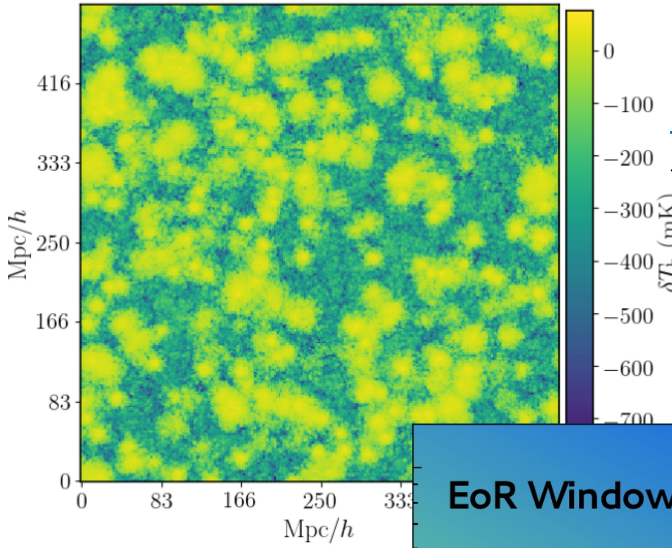
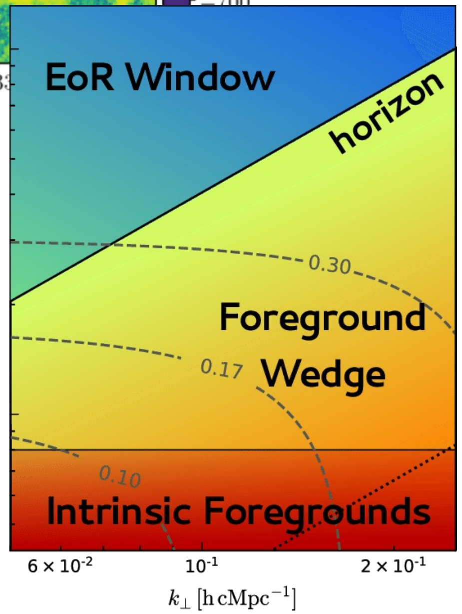
The SKA and 21-cm Cosmology

- 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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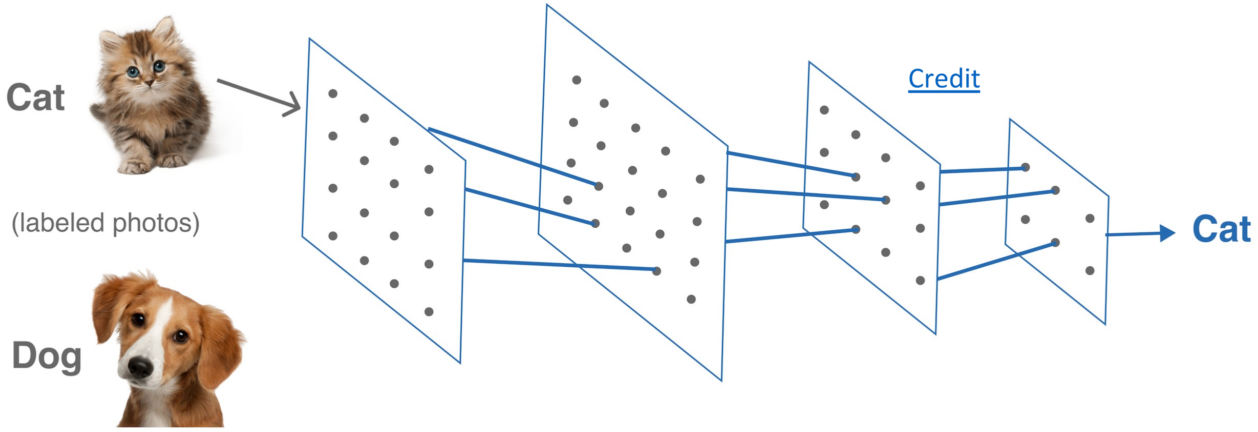
How do we emulate images?

- 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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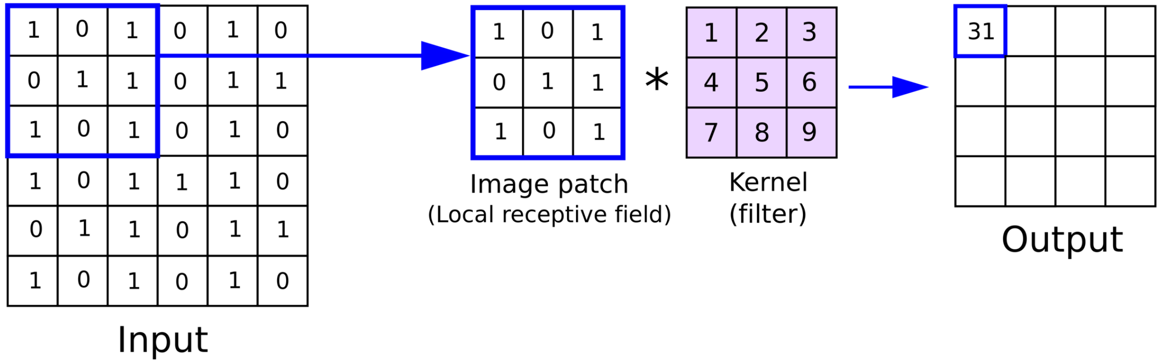
Convolutional Layers

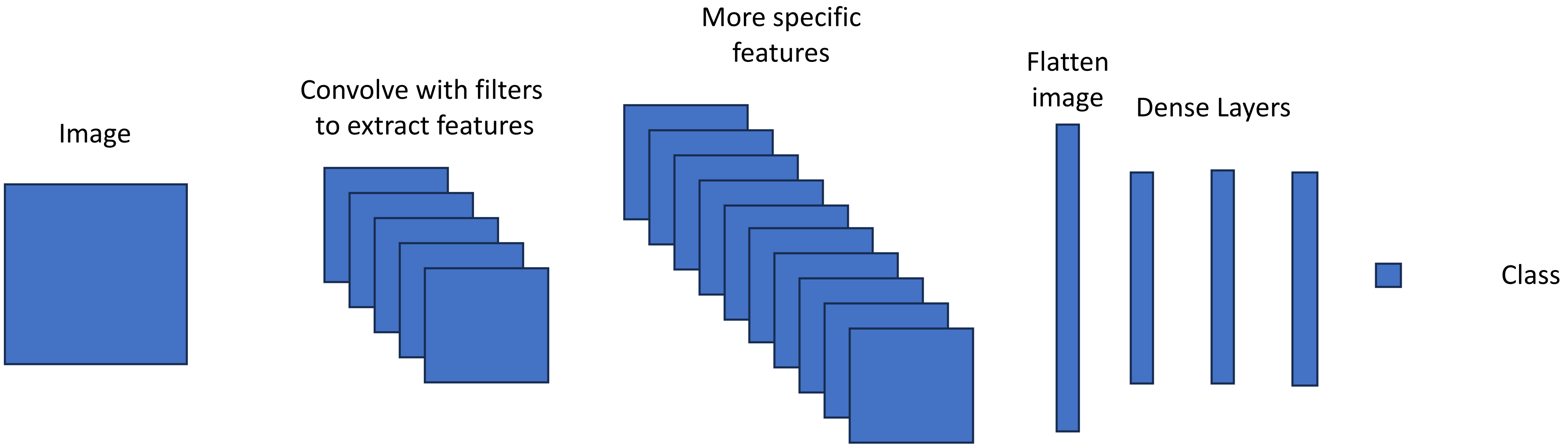
- Convolutional layers take an image and slide a filter across the image performing a dot product as they go

- Many filters are used to pick out key features gives you a stack of filtered images or a volume

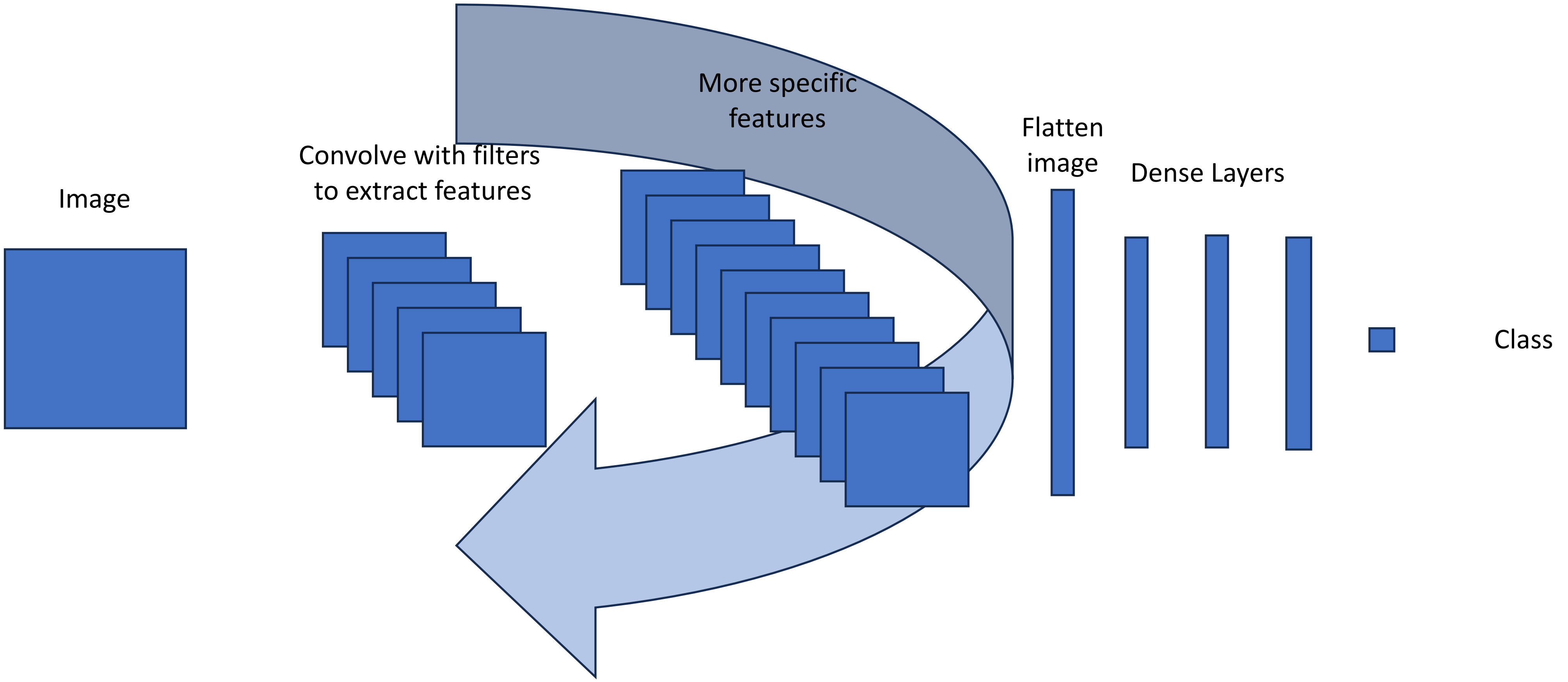
- Filters can be 2D or 3D in nature to increase or decrease the volume of the feature space at each layer



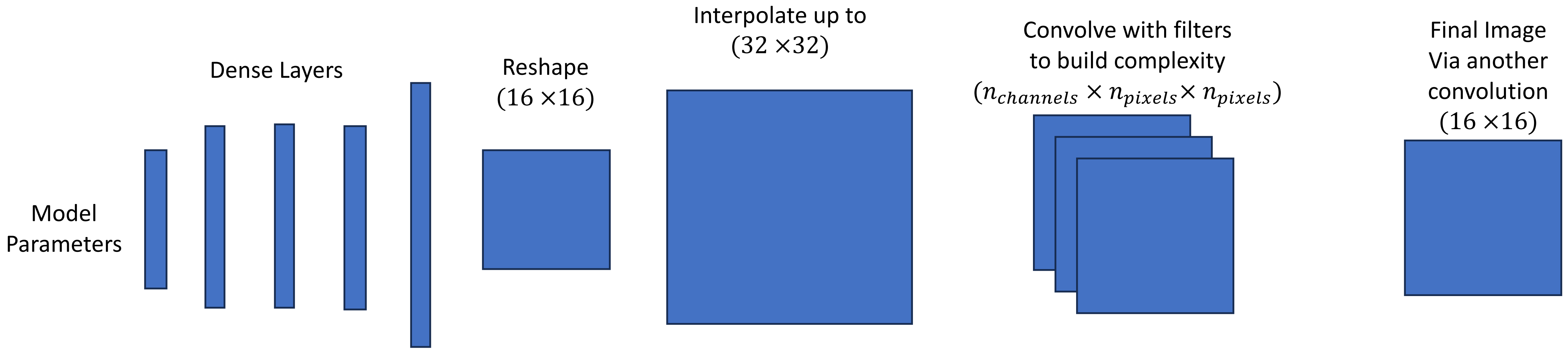
Convolutional Neural Networks



As Emulators

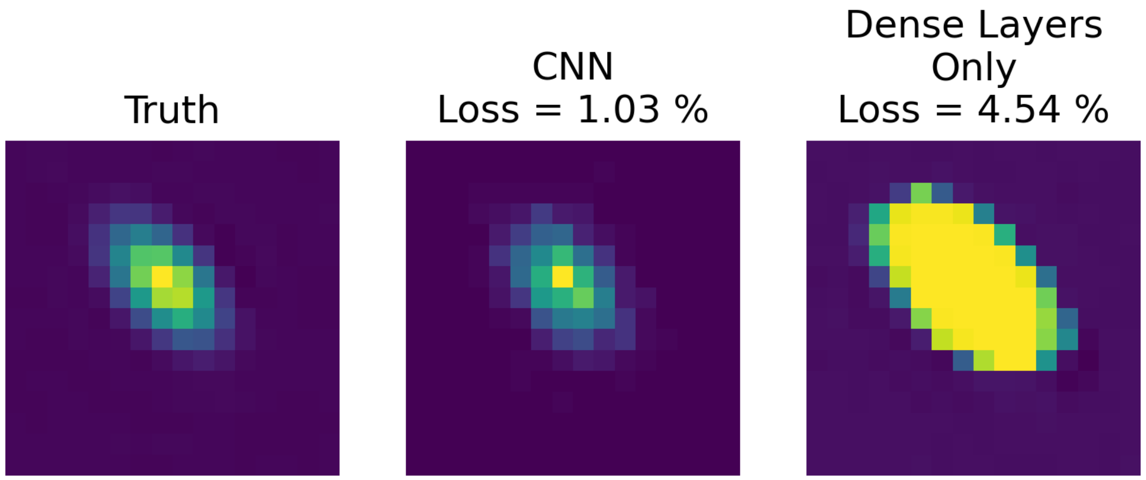


As Emulators



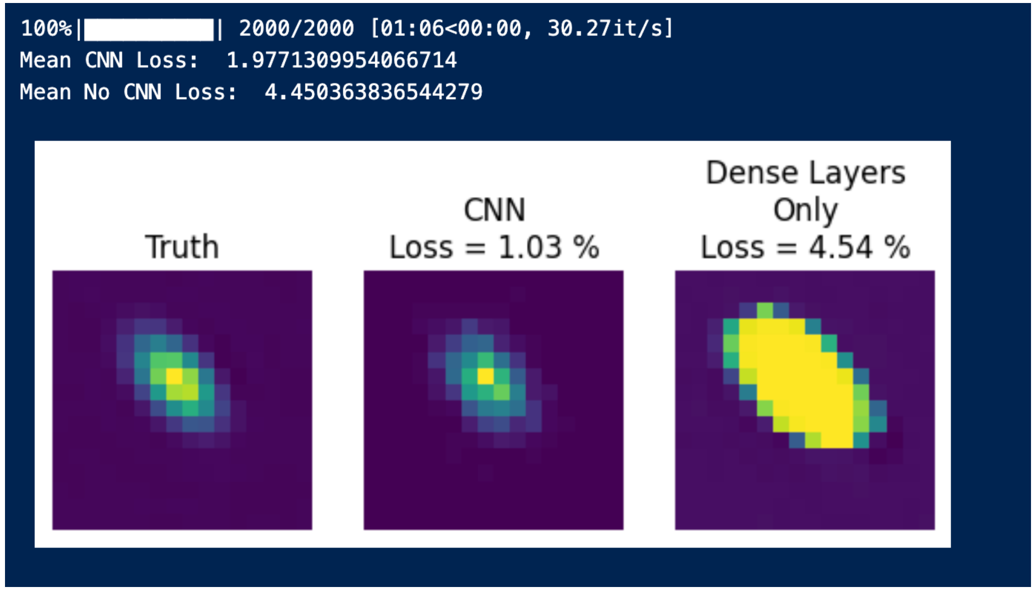
An Example

- 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



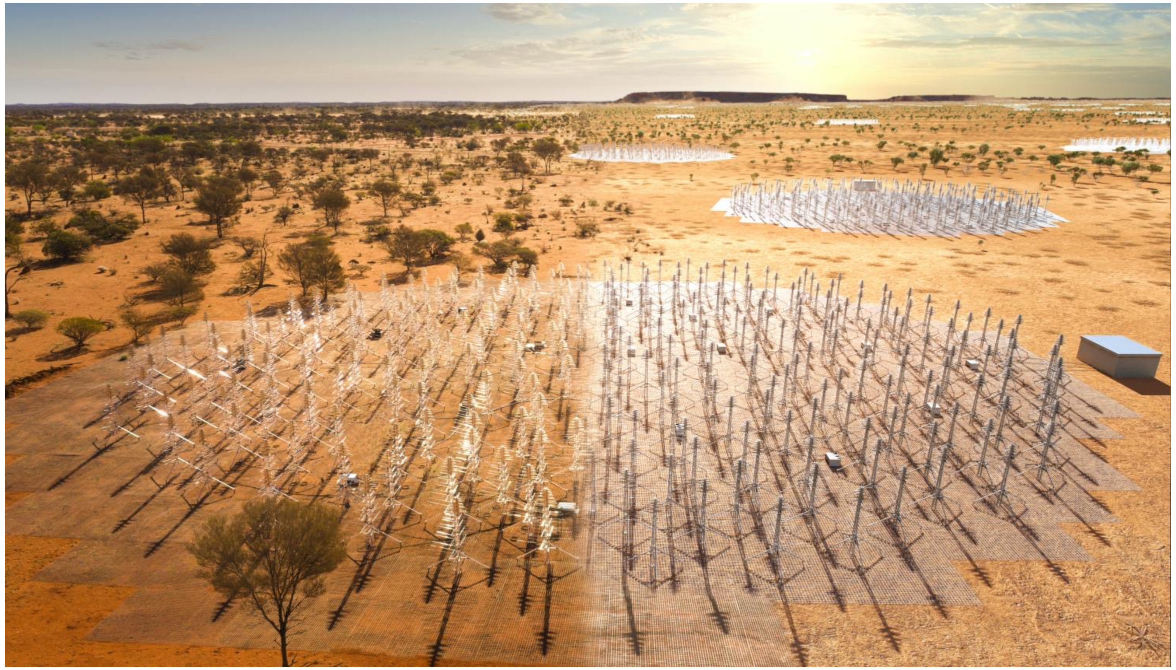
Optimisation

- 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



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

Next Lecture: Simulation Based Inference

- Why not just emulate the whole likelihood?