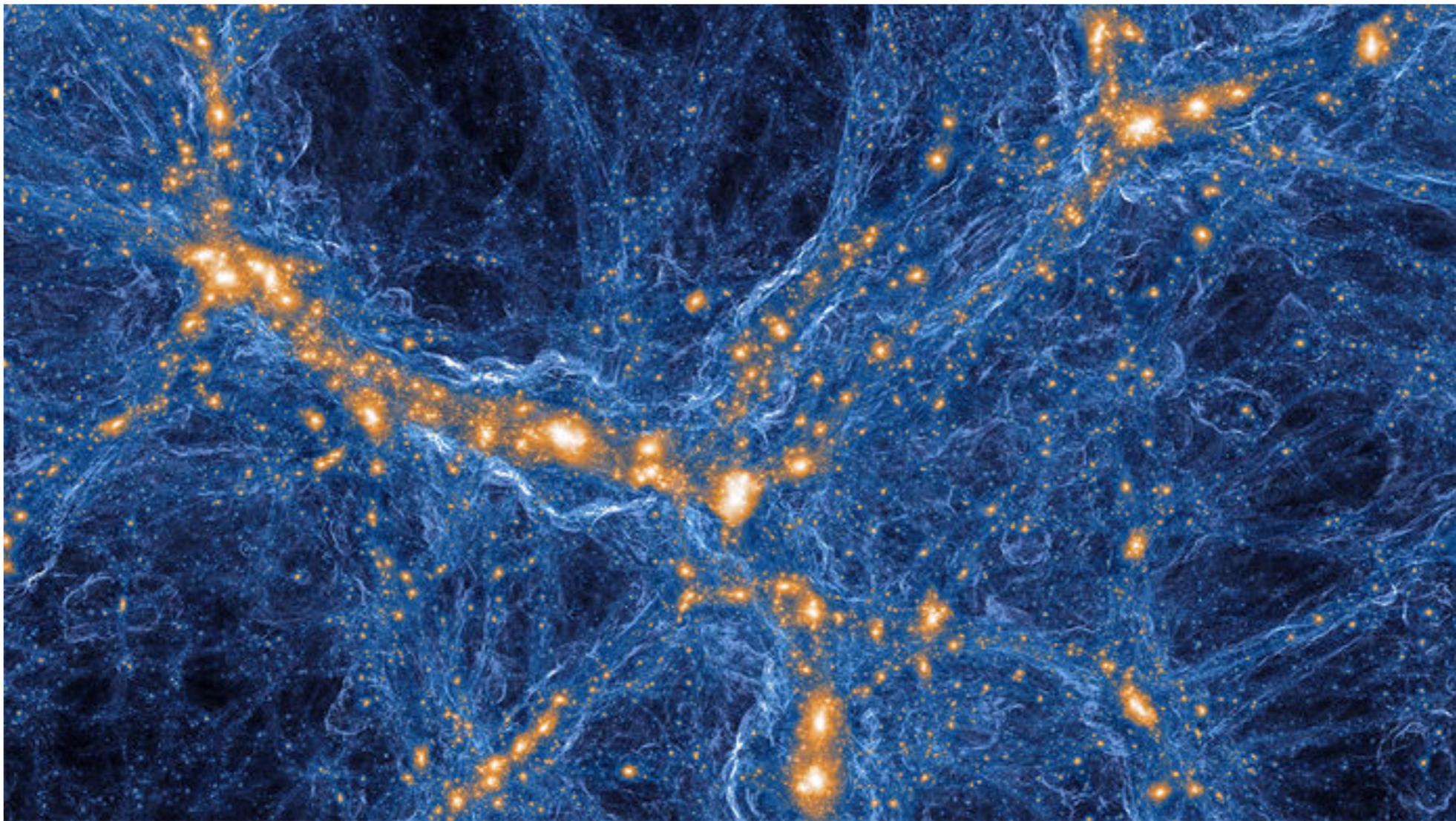




# Analysing the cosmic large scale structure with higher order statistics and machine learning

**Cristiano Sabiu (Yonsei University)**

With Xiao-Dong Li, Shuyang Pan, Miaoxin Liu, Jaime Forero-Romero, Ben Hoyle, Juhan Kim ++



**Machine Learning in Astronomy Seminar Series  
Western Sydney University - 28/04/2020**

# Contents

- ★ **Background Cosmology**
- ★ **Big Data Analytics and Graph Databases**
- ★ **Convolutional Neural Networks (CNN)**
- ★ **Conclusions**

# Background

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- \* The goal of modern cosmology is to **understand the physics** that governs our Universe on the largest scales
- \* Figure out the **constituents of the Universe**

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R - \Lambda g_{\mu\nu} = 8\pi GT_{\mu\nu}$$

# Background

---

- \* The goal of modern cosmology is to **understand the physics** that governs our Universe on the largest scales
- \* Figure out the **constituents of the Universe**

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R - \Lambda g_{\mu\nu} = 8\pi GT_{\mu\nu}$$

The game we play...

- 1) We start with Einstein's GR
- 2) Plug in a homogeneous/isotropic metric
- 3) Plug in energy/matter components
- 4) Obtain evolution equations for:
  - **Expansion of the Universe**
  - **Growth of density perturbations**

# Background

---

- \* What causes cosmic acceleration?
  - Vacuum energy or Scalar field(s)?
  - Or something more strange\*?!
    - \* (if that's not strange enough)
- \* What is Dark Matter?
  - Is it Self-interacting?
  - Is it Decaying?

Each of the above possibilities could effect

- Universe expansion
- Clustering of matter

# Background

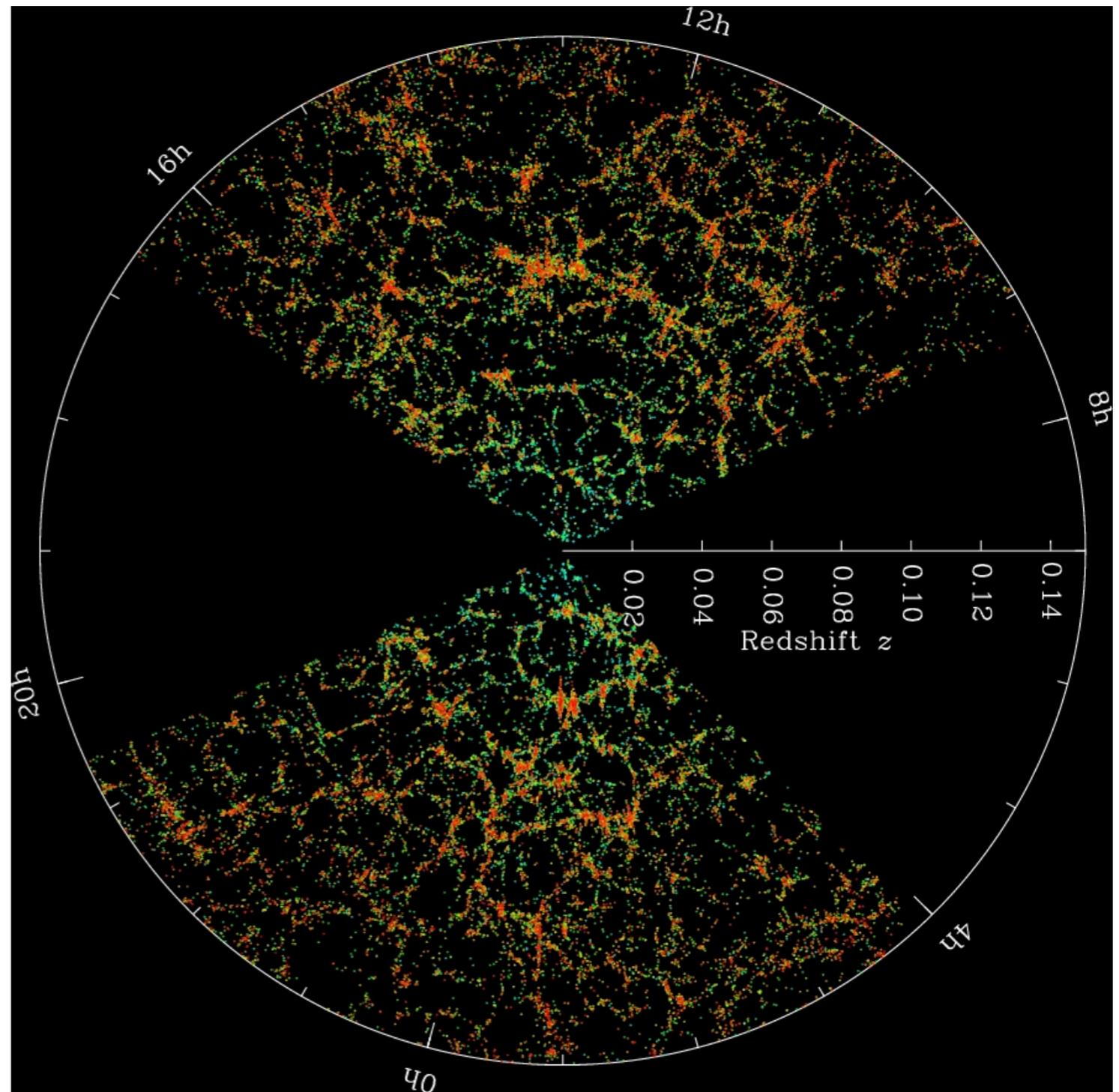
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We can now map large volumes of the Universe in 3D using galaxies as tracers of the underlying matter potential

But then what do we do with all these galaxy positions?



SDSS

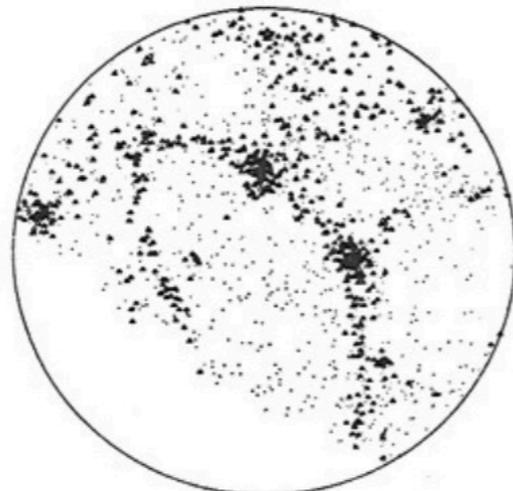


# Background

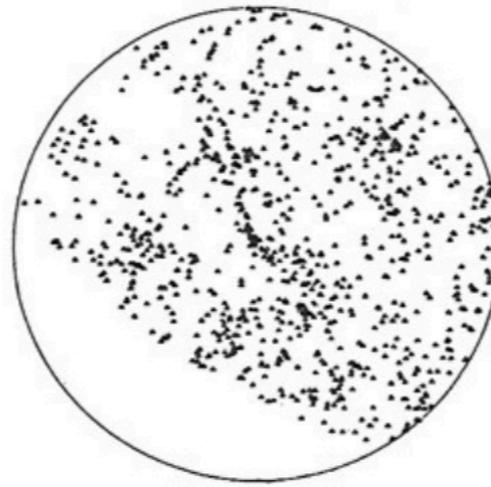
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## N-body Simulations

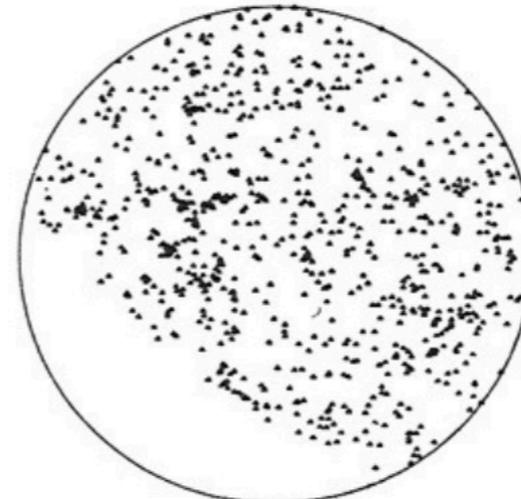
1980s  
~1000 particles



HDM



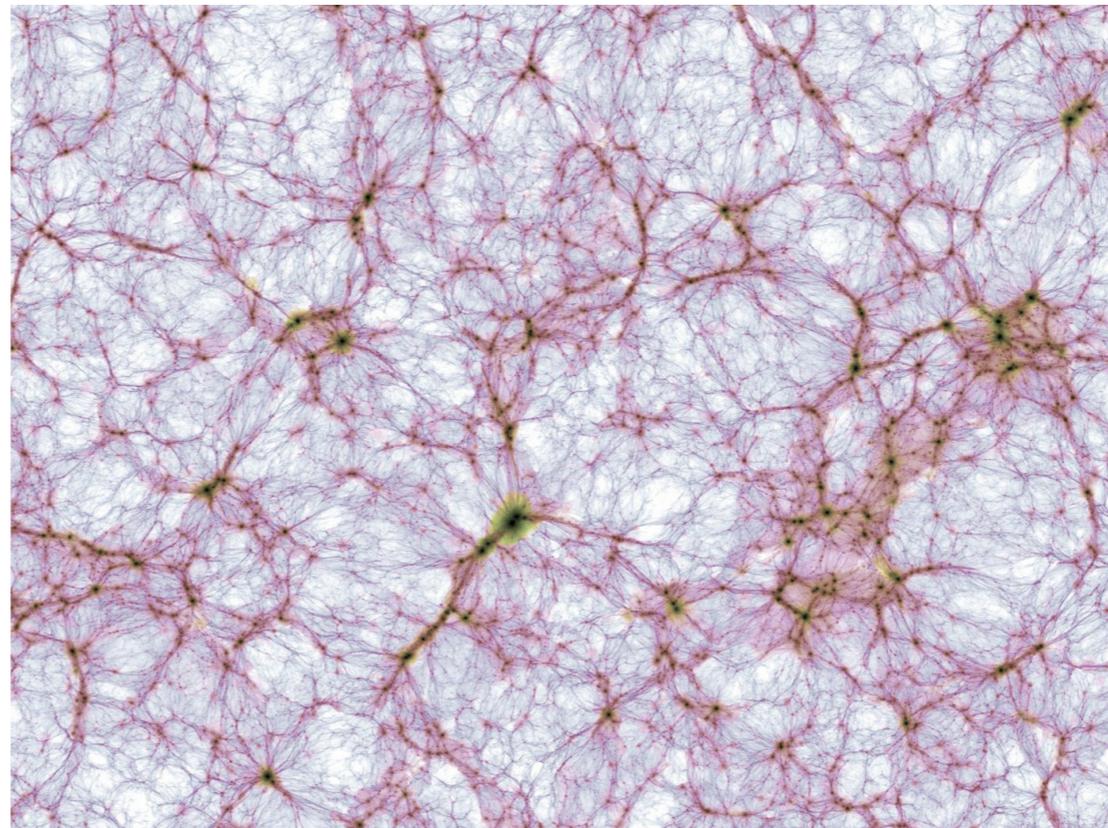
Observed Galaxy Distribution



CDM

Credit: S. D. M. White, 1986

Today  
~10,000,000,000 particles



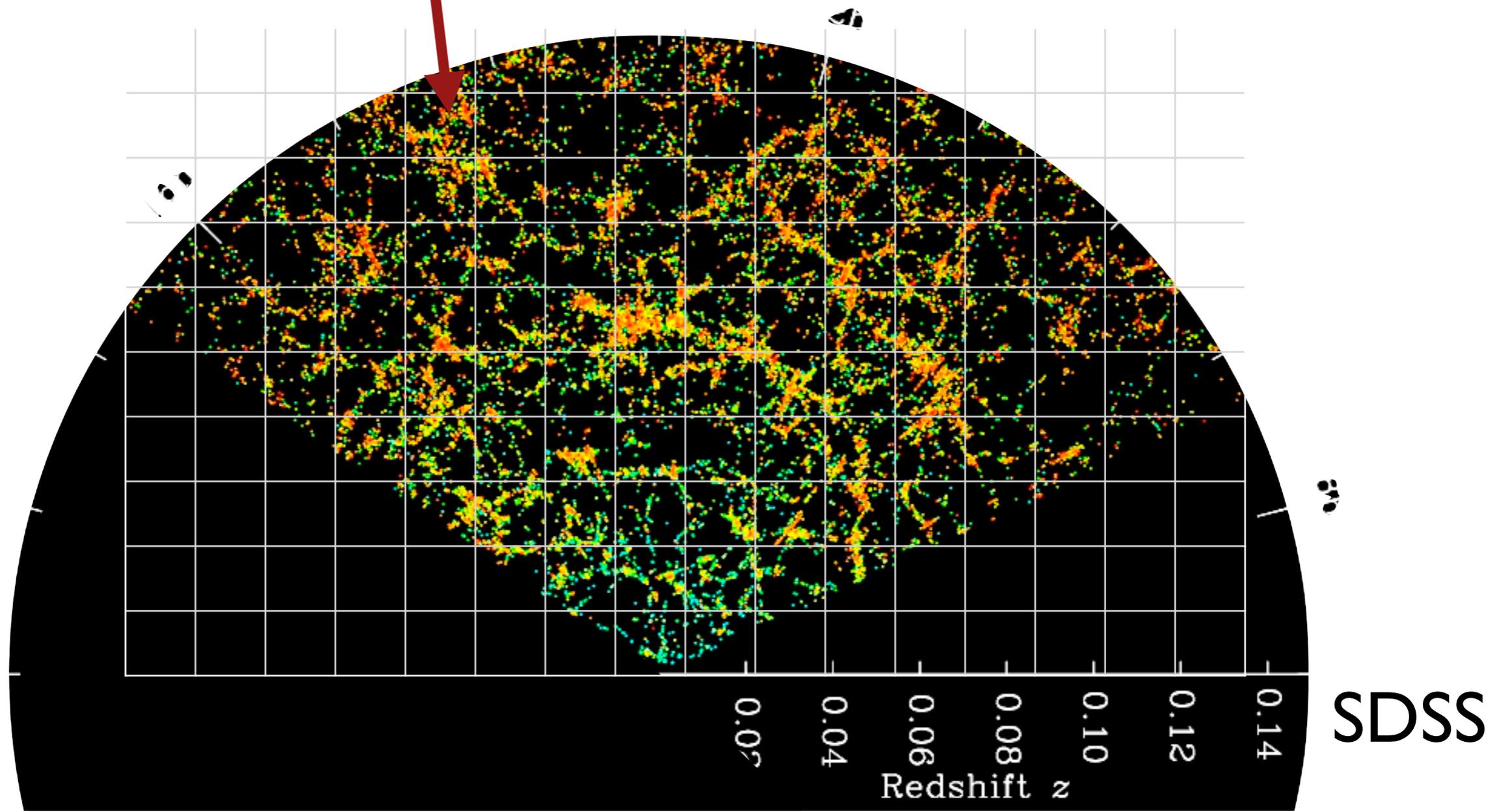
Illustris TNG  
Simulation

# Background

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Count galaxies in cells and compute:

$$\xi(r) = \langle \delta(x)\delta(x+r) \rangle_x$$



# Background

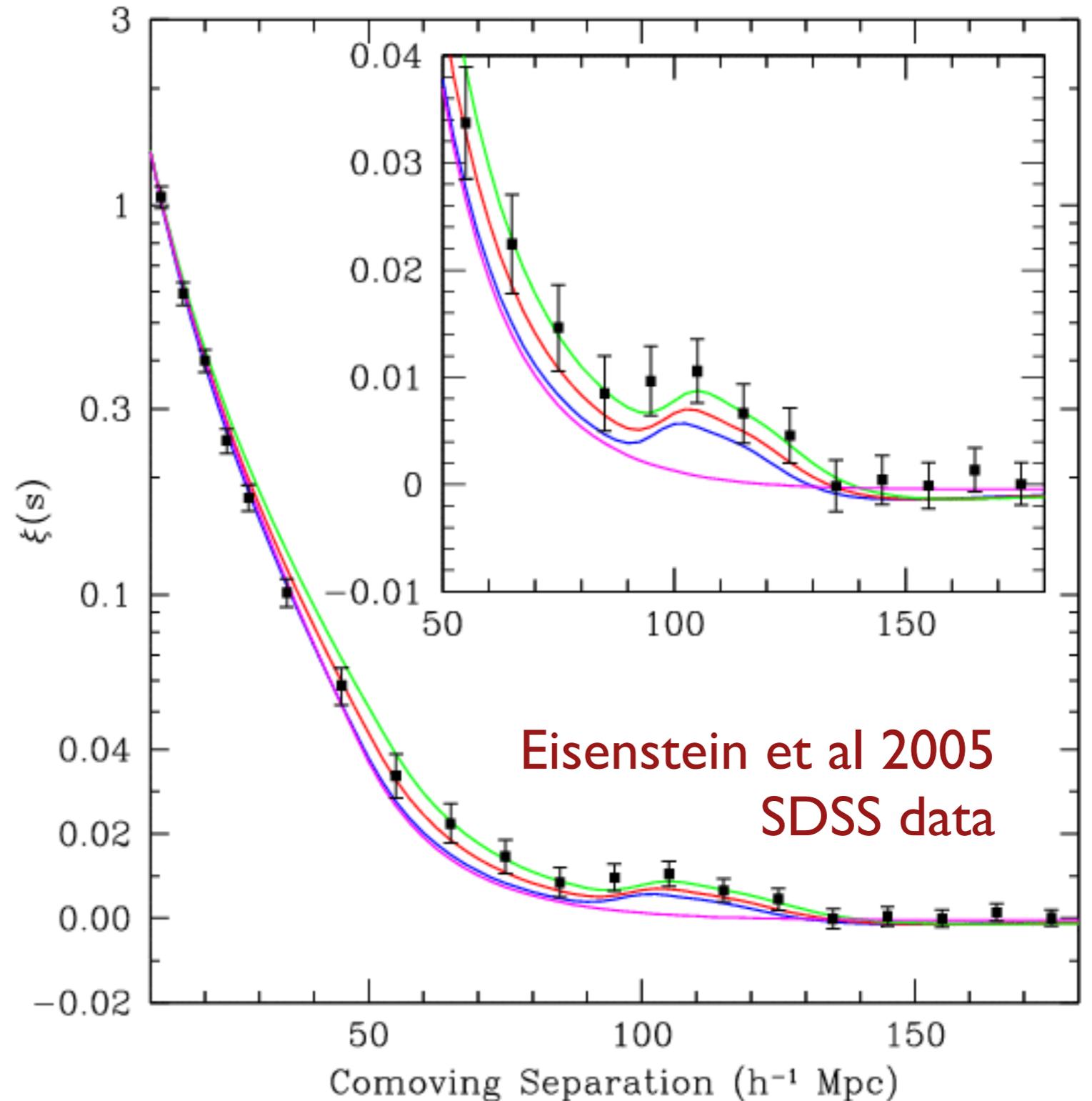
The measured  
2-point correlation  
function (**2PCF**)

Large clustering strength  
at **small separations**

Almost zero on  
scales  $> 200\text{Mpc}/h$

We can compare  
observation and theory/  
simulations with the 2PCF

Recently some groups  
have used ML...



# Background

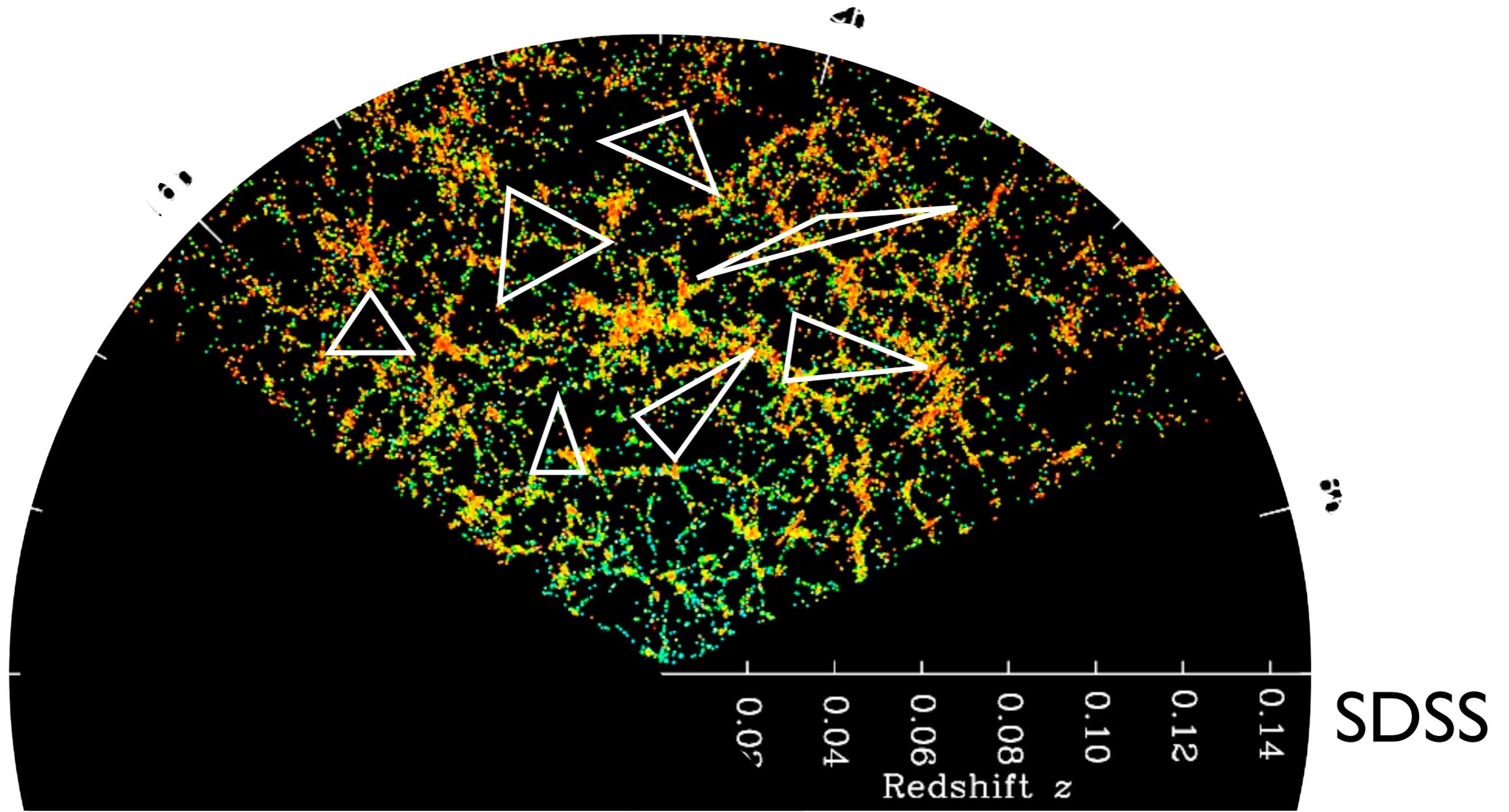
---

We can try to measure higher order statistics

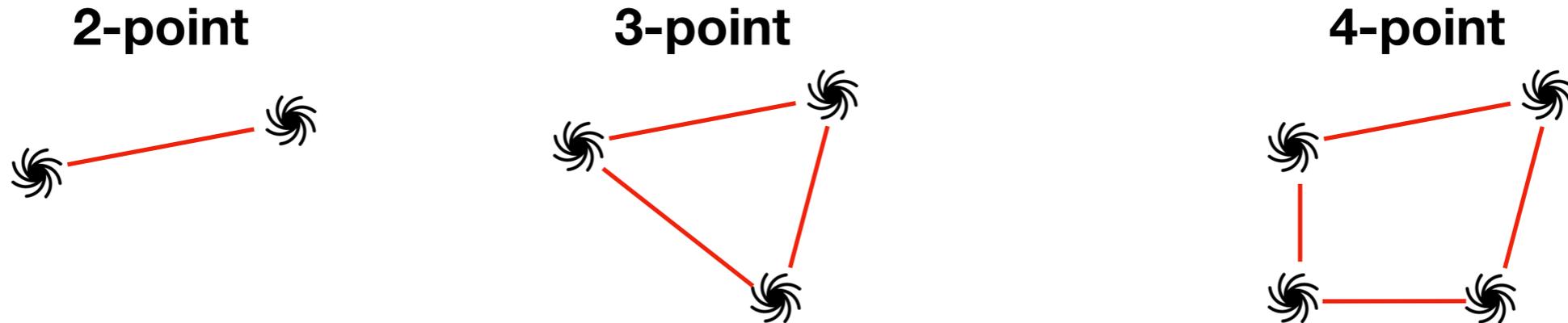
$$\zeta(r_1, r_2, r_3) = \langle \delta_1 \delta_2 \delta_3 \rangle$$

Naively:

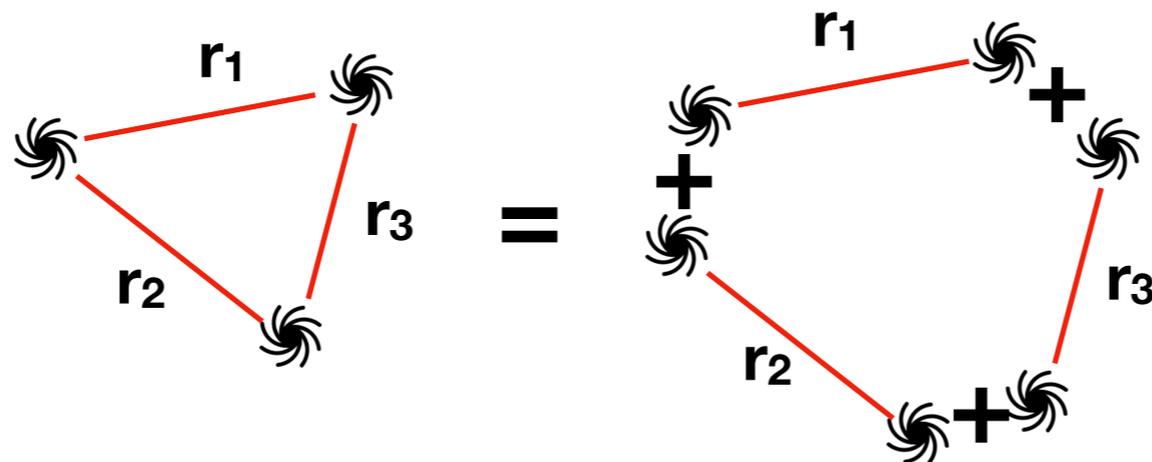
- Counting Pairs requires  $N^2$  calculations
- Counting Triplets requires  $N^3$  calculations



# Graph Database solution for Galaxy Clustering statistics



- The computationally expensive part of measuring higher order statistics is in making sure the distances between data points satisfy our specific criteria i.e.  $r_1$ ,  $r_2$ ,  $r_3$ , etc
- However we notice that all higher order statistics are just complex combinations 2-point statistics



So rather than treat data positions as the important feature, rather treat each data pair (relationship) as the main information!

# Graph Databases

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A graph within graph databases is based on graph theory.

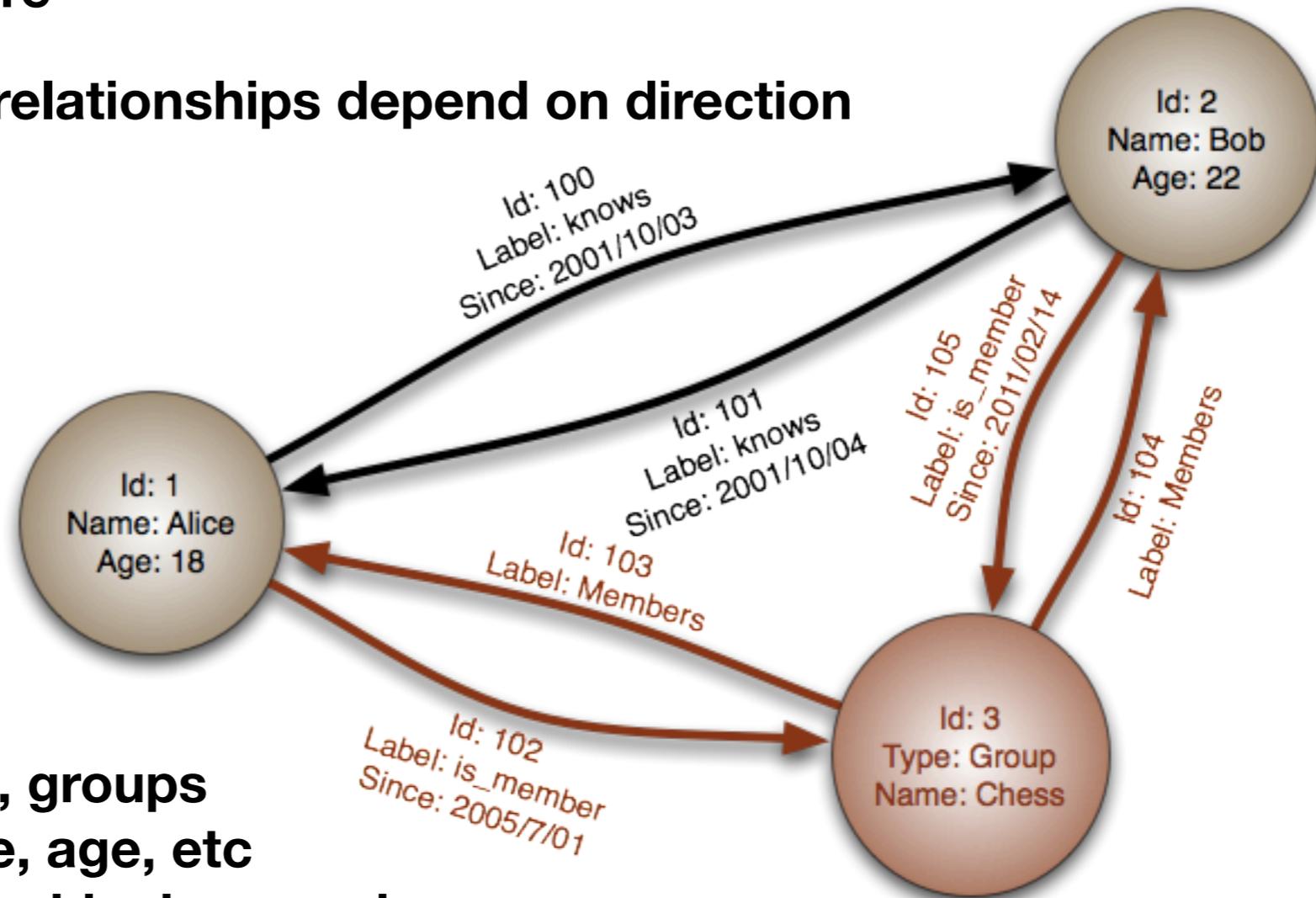
- **Nodes** represent entities or instances such as people, businesses, accounts, or any other item to be tracked. They are roughly the equivalent of the record, relation or row in a relational database, or MySQL item
- **Relationships**, are the lines that connect nodes to other nodes; representing the relationship between them. Meaningful patterns emerge when examining the connections and interconnections of nodes, properties and relationships. Relationships are the key concept in graph databases, representing an abstraction that is not directly implemented in a relational model like SQL
- **Properties** are germane information to nodes. For example, if *Wikipedia* were one of the nodes, it might be tied to properties such as website, reference material, or words that starts with the letter *w*, depending on which aspects of Wikipedia are germane to a given database.

# Graph Databases

---

In 2009 Facebook gave up using their MySQL storage and moved to a graph structure

A directed graph: relationships depend on direction



Nodes: people, places, groups

Node properties: name, age, etc

Relationships: membership, known since

Graph for our purposes will be much simpler!

# Graph Database solution for Galaxy Clustering statistics

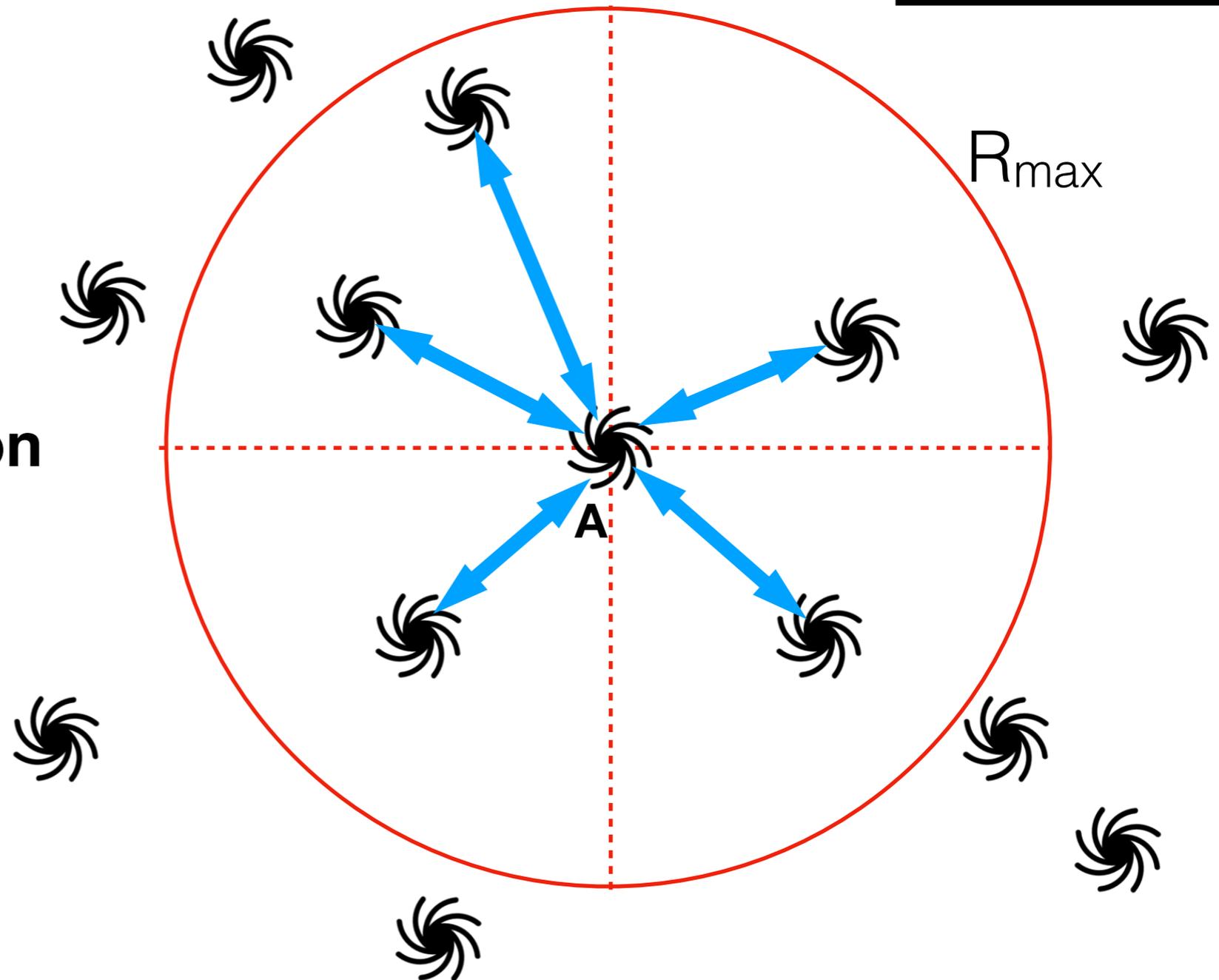
Each galaxy (or random) point is a **node** which may have relationships to there nodes

For our purposes the relationship information is the distance to neighbours within  $R_{max}$

Neighbour list can be obtained quickly using a **kd-tree** algorithm

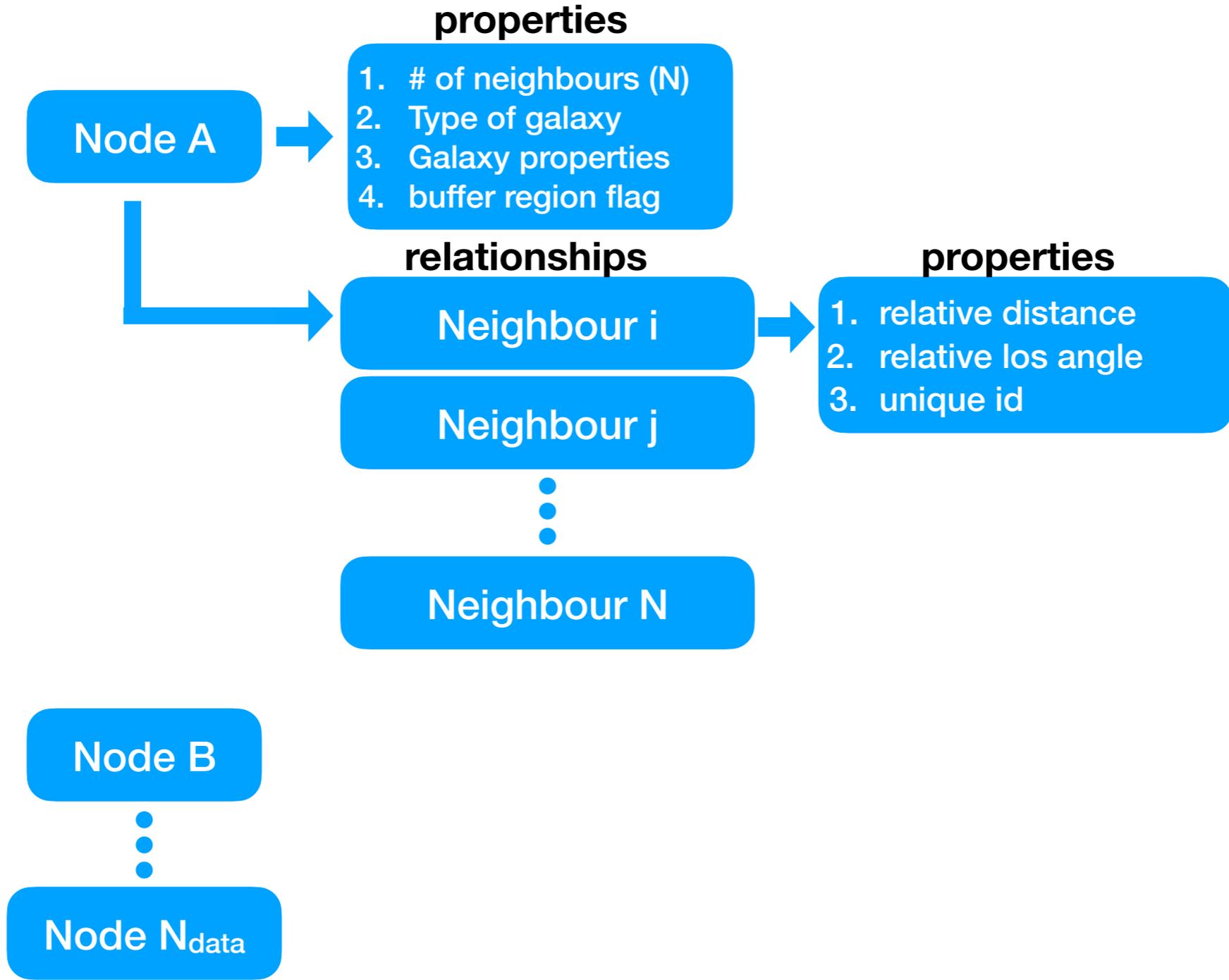
This is a Node

Relationship



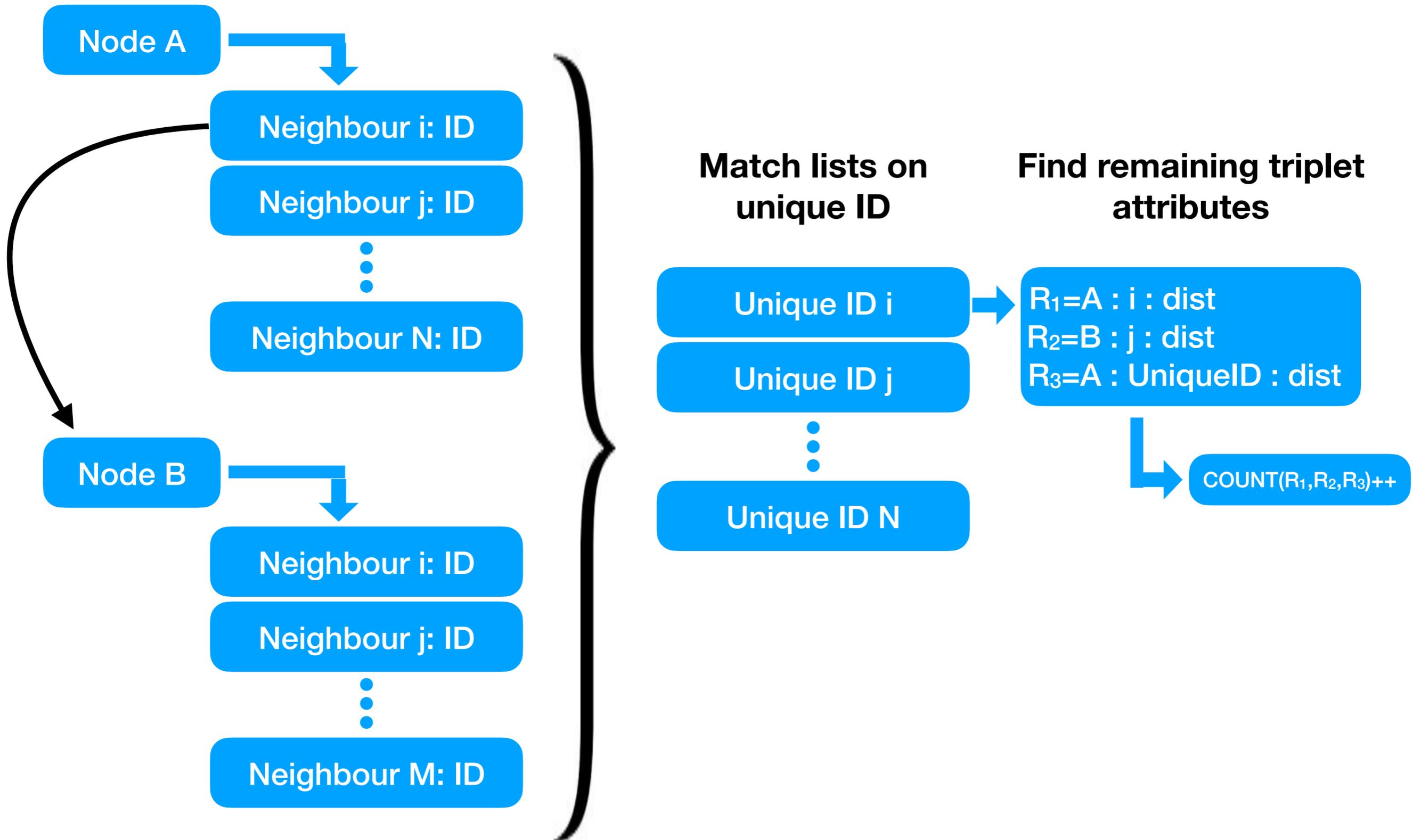
# Graph Database solution for Galaxy Clustering statistics

## Graph Database Structure



# Graph Database solution for Galaxy Clustering statistics

## Query Graph: 3PCF



# Graph Database solution for Galaxy Clustering statistics

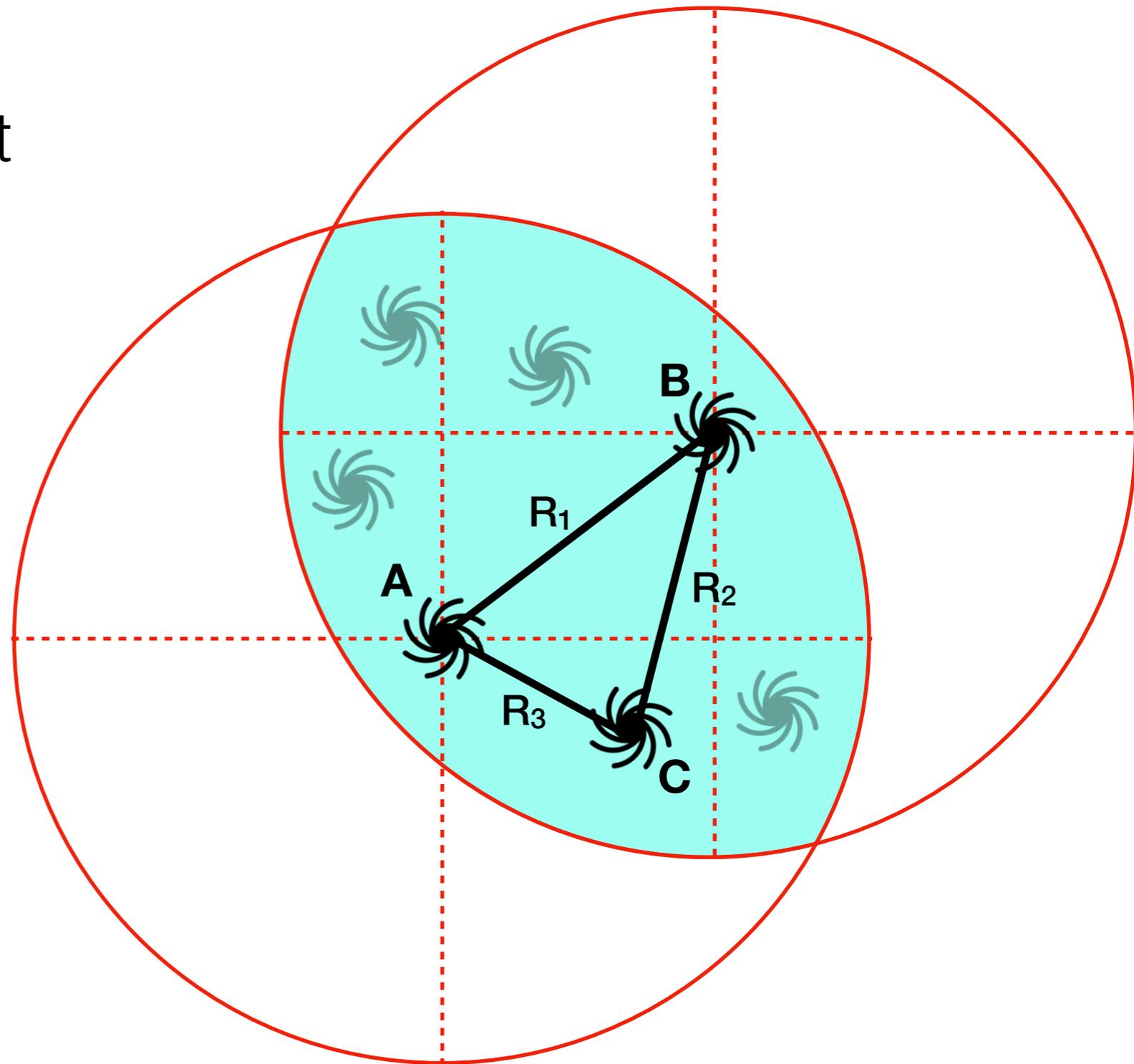
## Query Graph: 3PCF

The intersection of two sets (**A, B**) contains a list of points, **C**, that will complete the triangle A,B,C such that,

$$0 < R_1, R_2, R_3 < R_{\max}$$

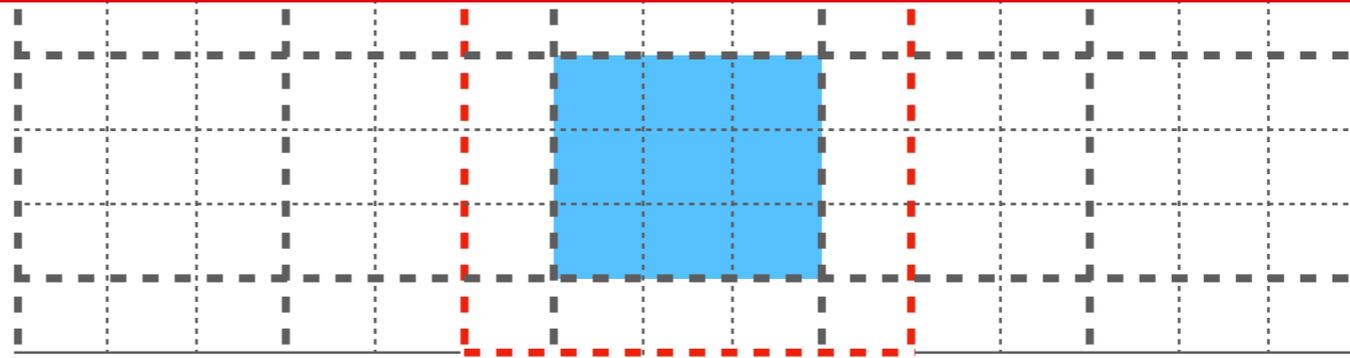
The intersection must be computed  $\sim N^2$  times!

For 2 **ordered lists**, the intersection can be computed very quickly!

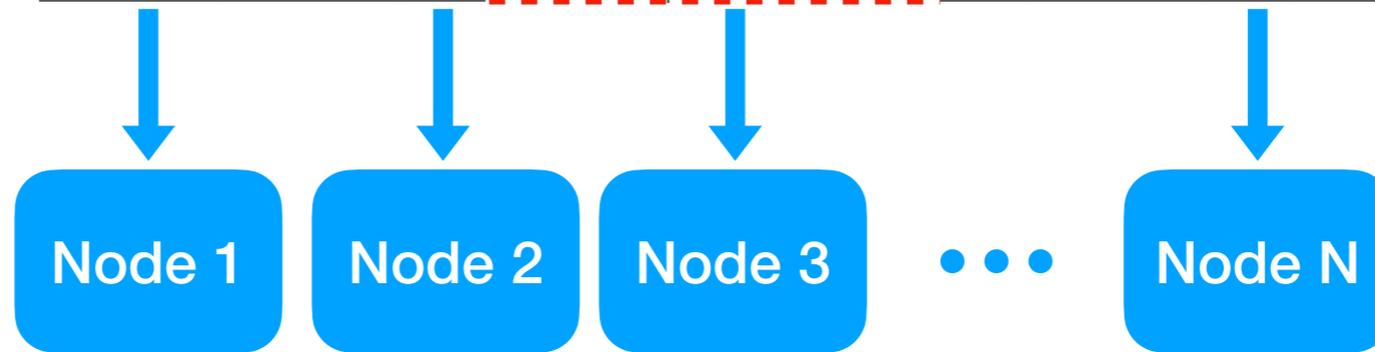


# Graph Database solution for Galaxy Clustering statistics

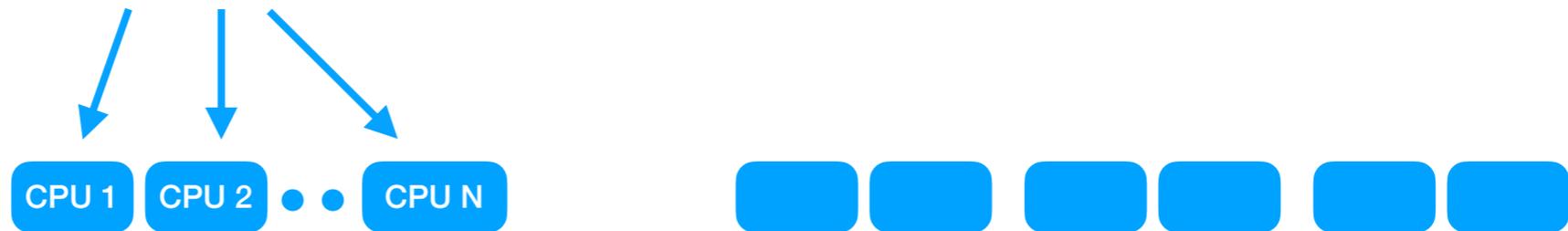
Domain decomposition is precomputed



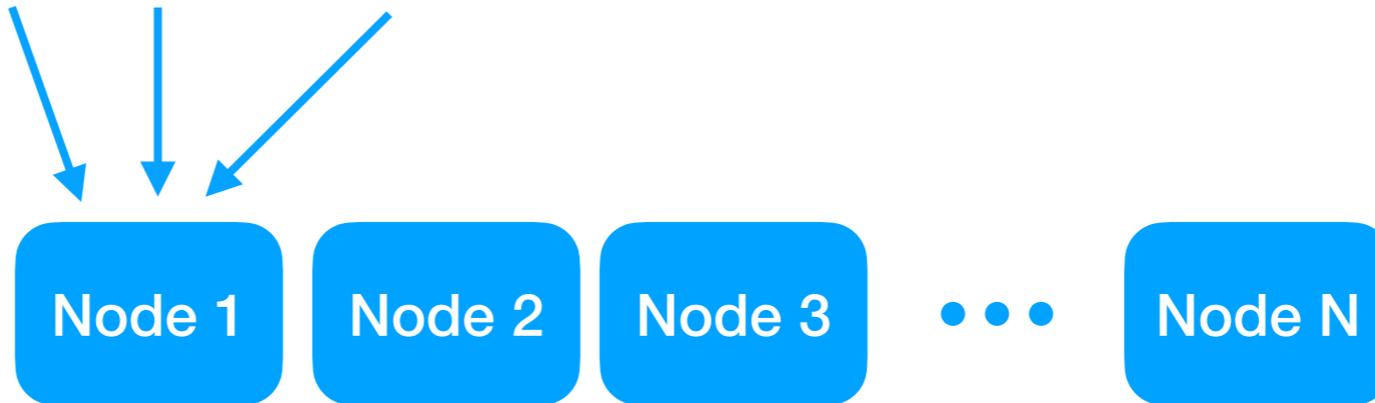
Spawn  $N$  MPI processes



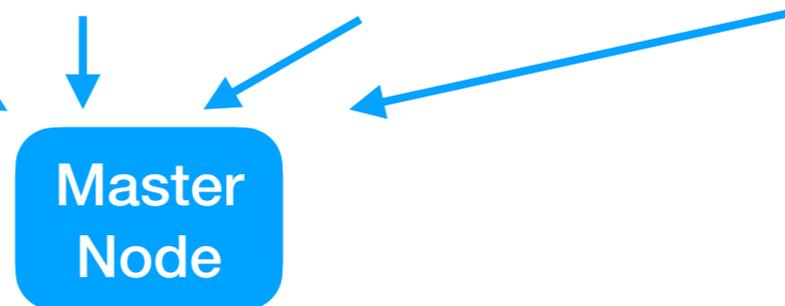
OpenMP threading



Reduce OMP arrays for each node/domain

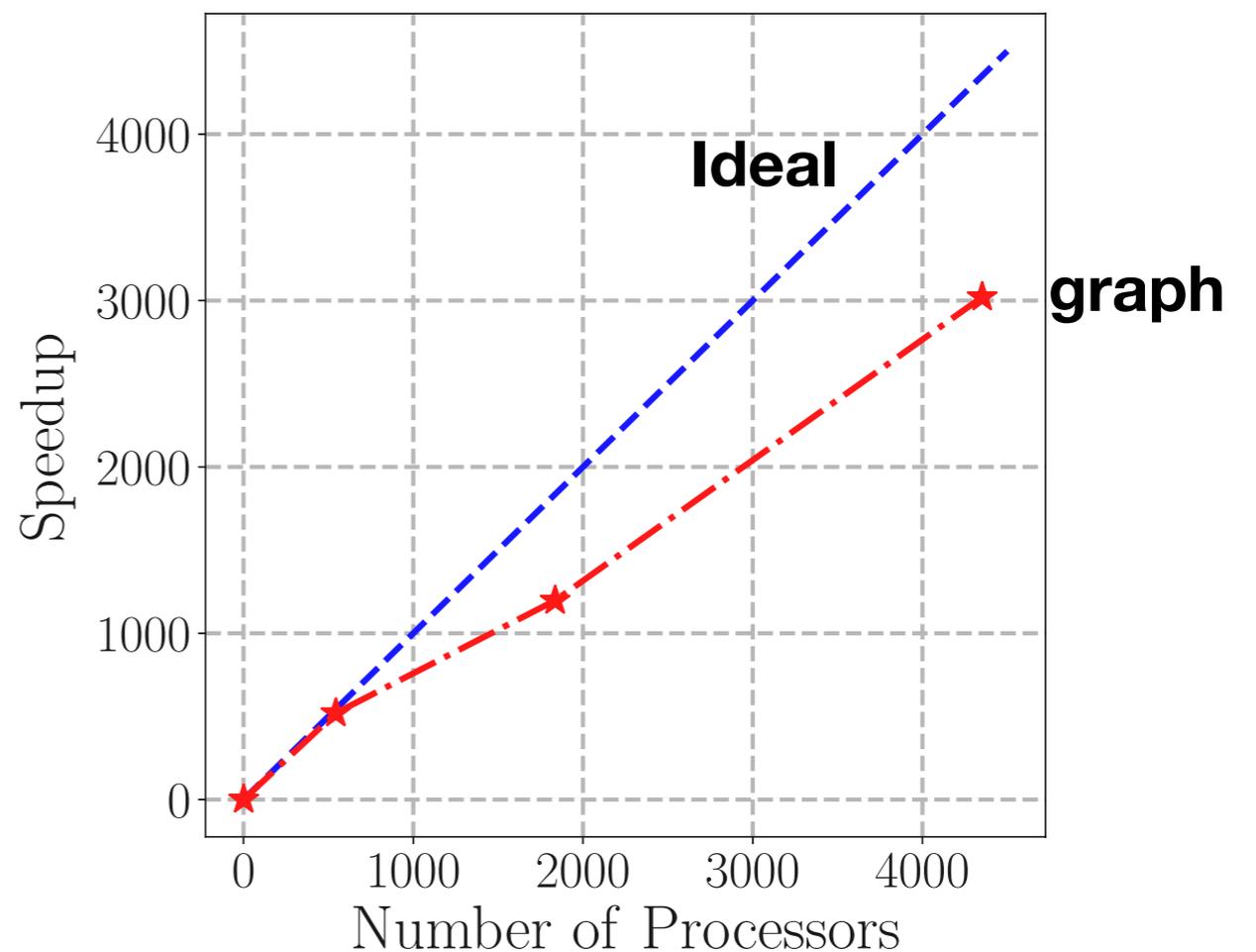
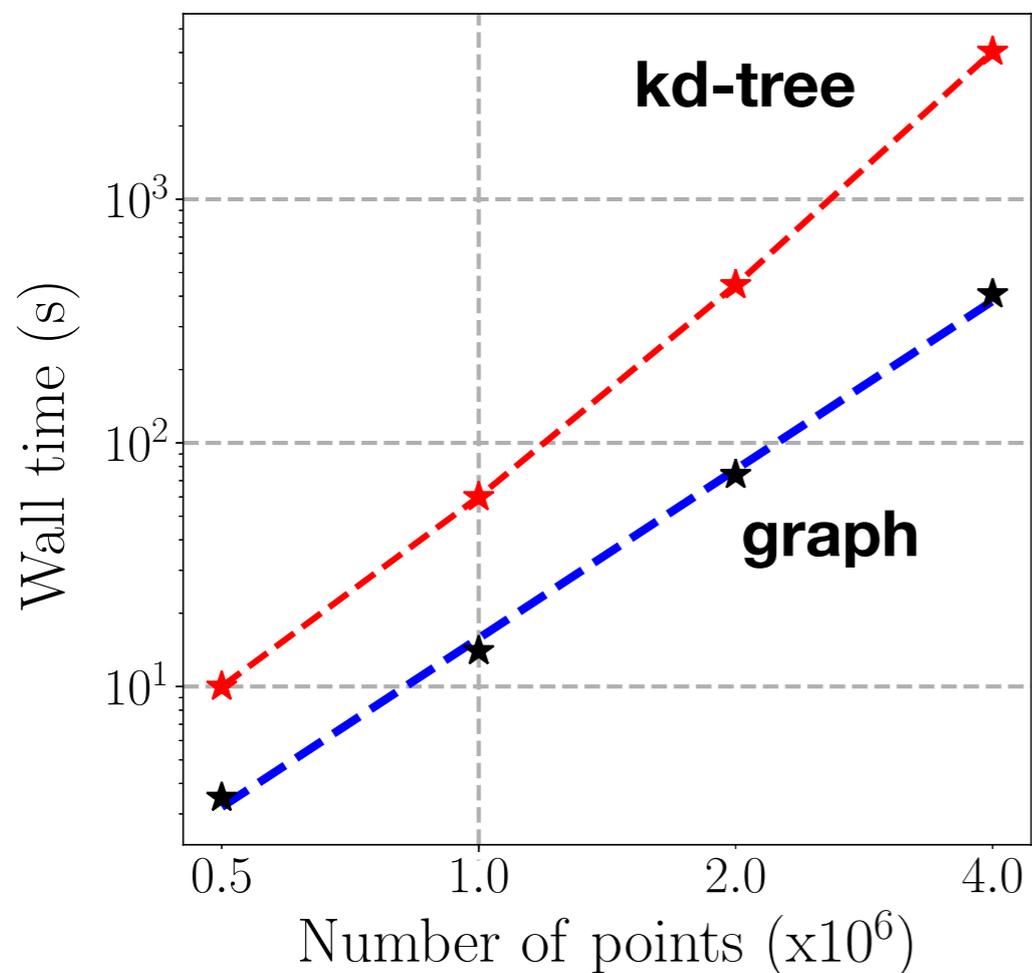


Collect MPI arrays and output



# Graph Database solution for Galaxy Clustering statistics

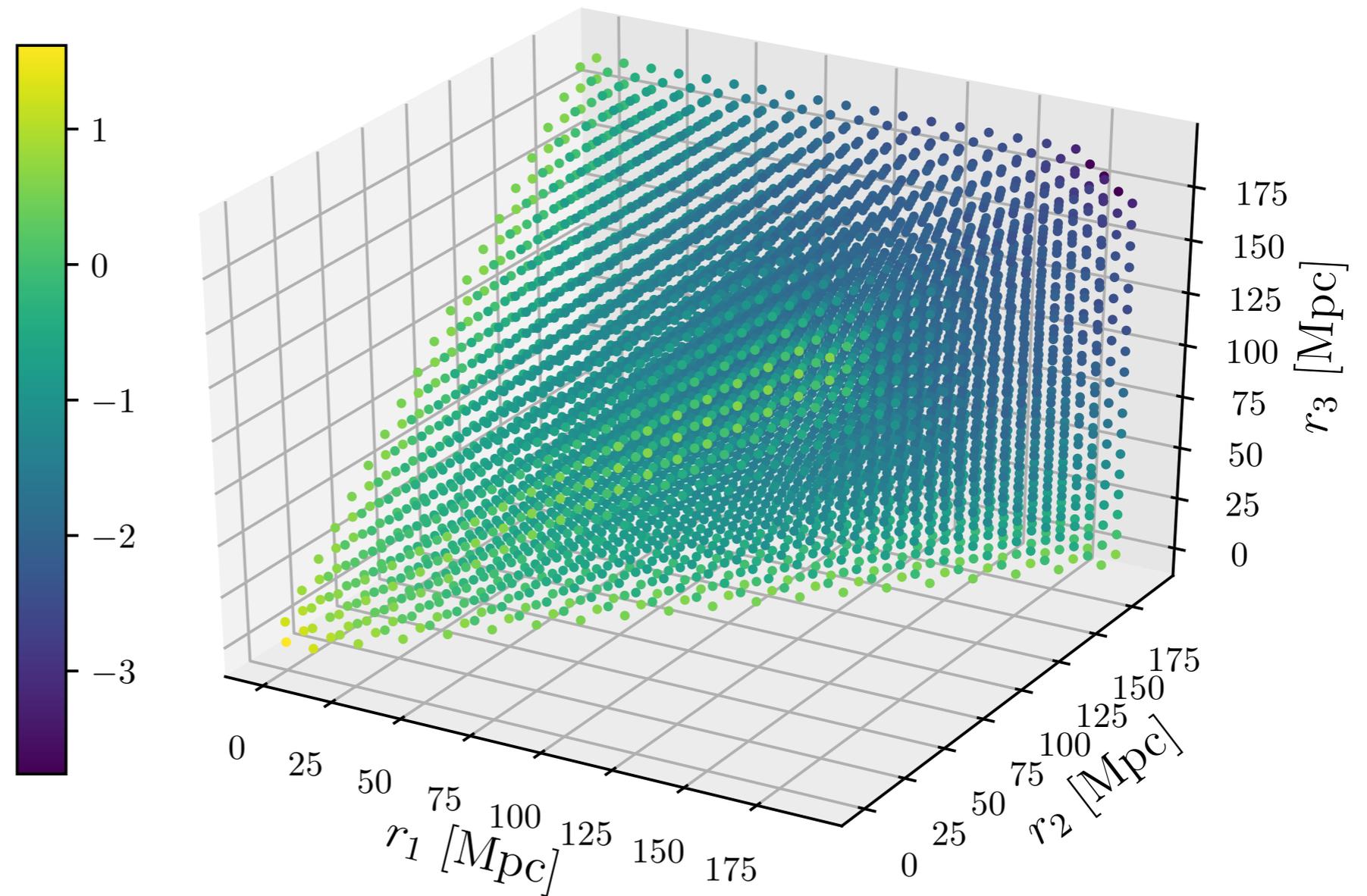
## Benchmarking



★ C. Sabiu, B. Hoyle, J. Kim, X-D Li  
★ <https://arxiv.org/abs/1901.00296>

# Graph Database solution for Galaxy Clustering statistics

Taking the SDSS CMASS  
DR12 galaxies ( $\sim 1\text{M}$ )



★ C. Sabiu, B. Hoyle, J. Kim, X-D Li

★ <https://arxiv.org/abs/1901.00296>

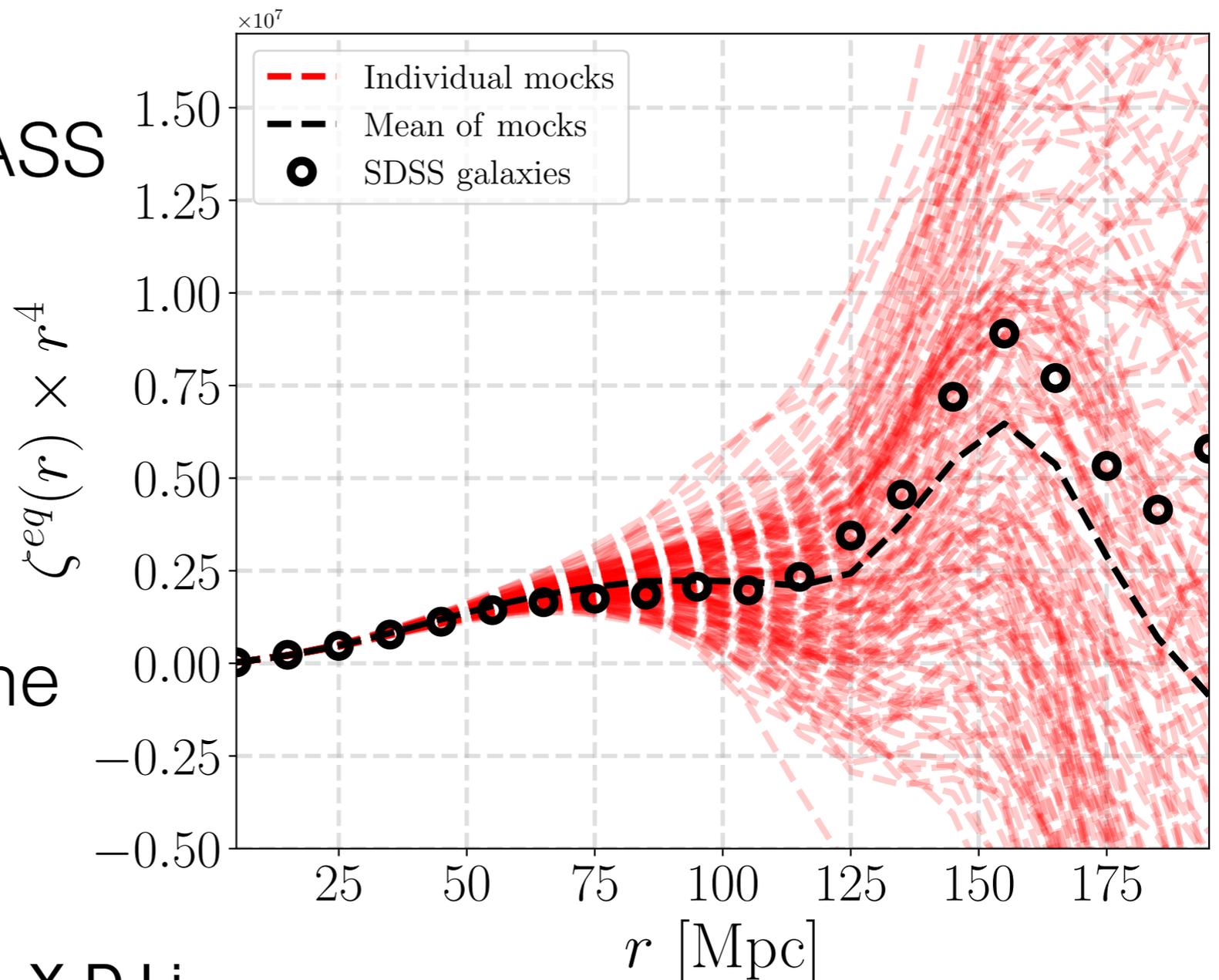
# Graph Database solution for Galaxy Clustering statistics

## BAO in the 3-point function

Taking the SDSS CMASS DR12 galaxies ( $\sim 1\text{M}$ )

We look at equilateral triangles

We see evidence of the BAO peak



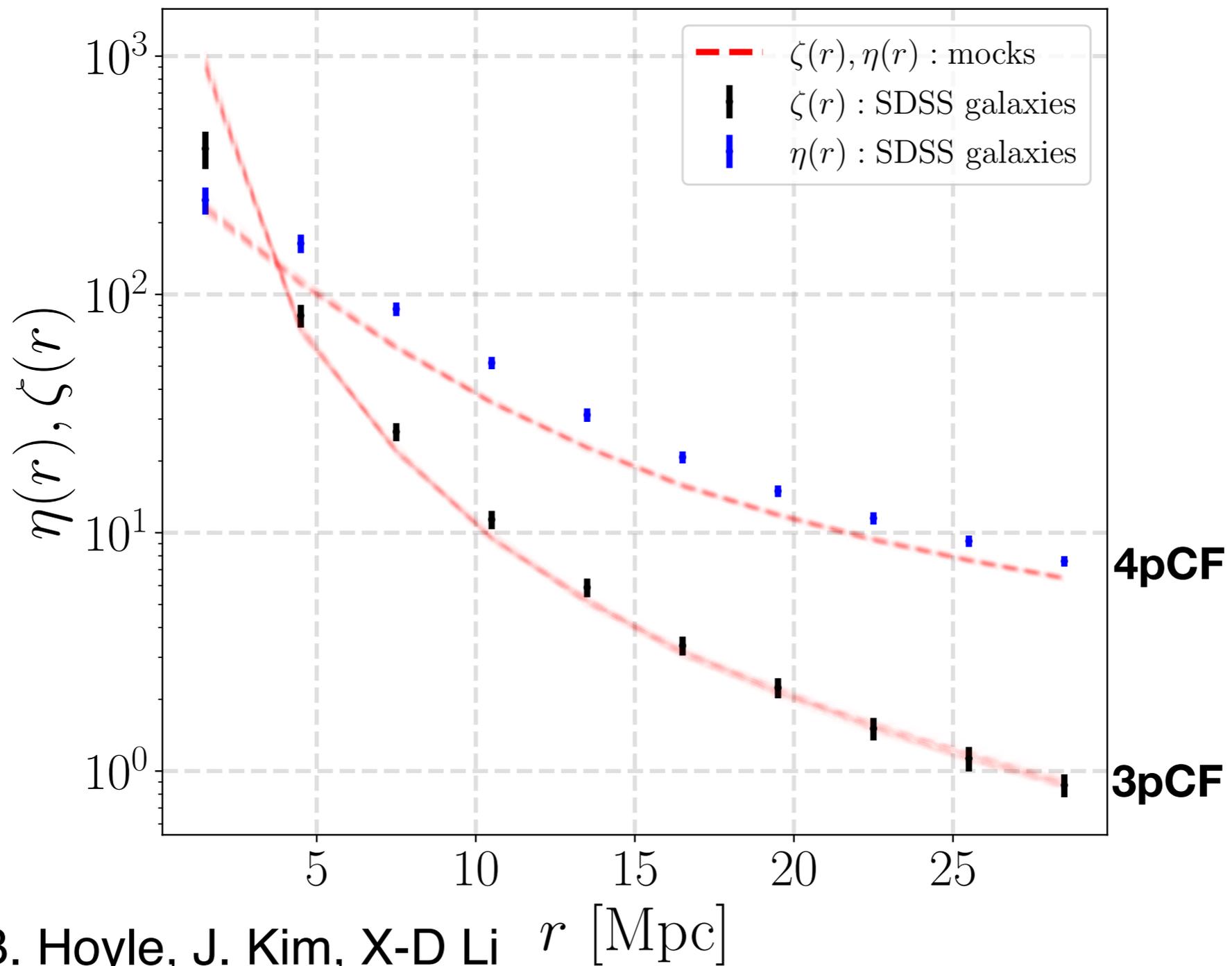
★ C. Sabiu, B. Hoyle, J. Kim, X-D Li

★ <https://arxiv.org/abs/1901.00296>

Isotropic, equilateral 3PCF

# Graph Database solution for Galaxy Clustering statistics

## 4-point correlation function

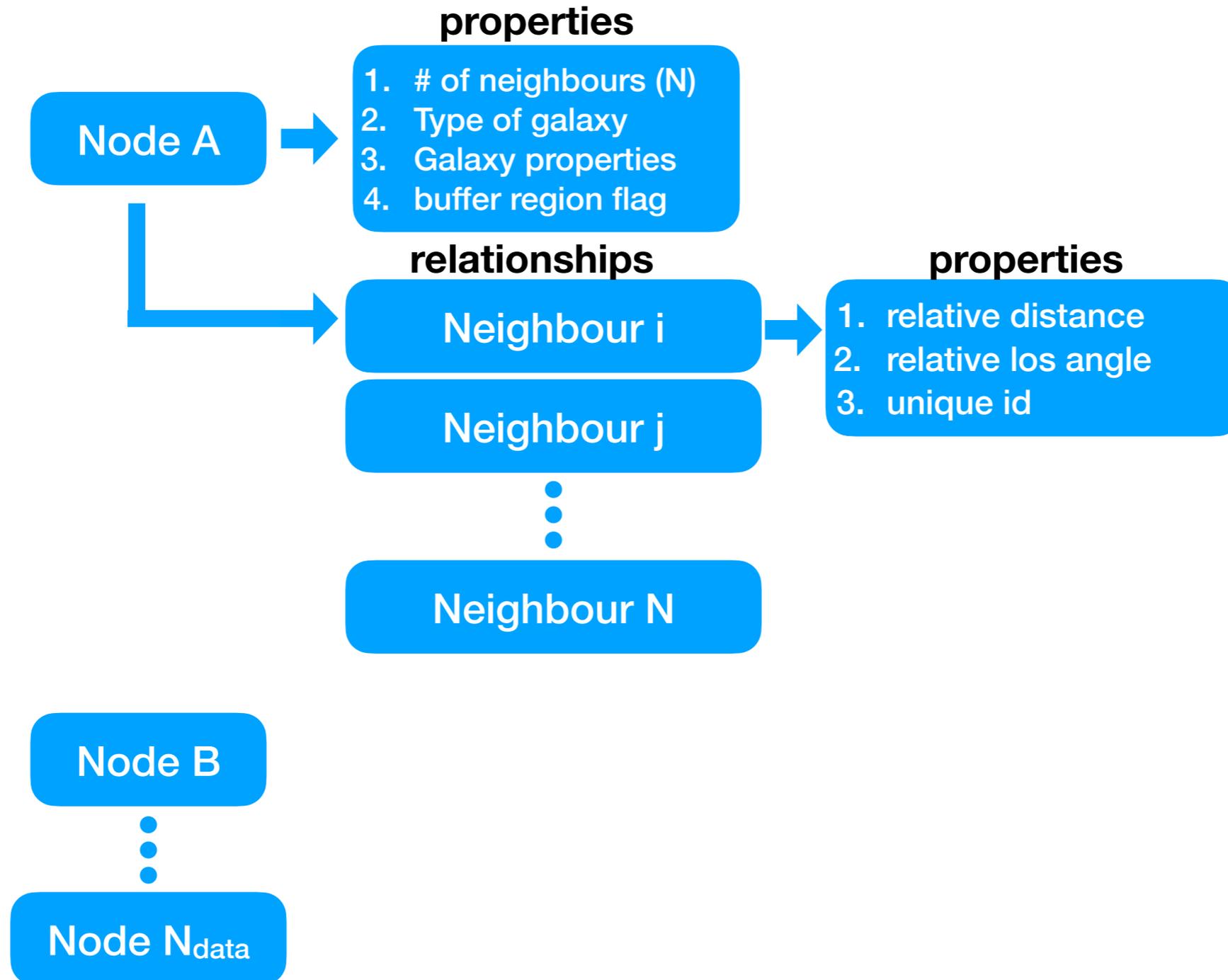


★ C. Sabiu, B. Hoyle, J. Kim, X-D Li  $r$  [Mpc]

★ <https://arxiv.org/abs/1901.00296>

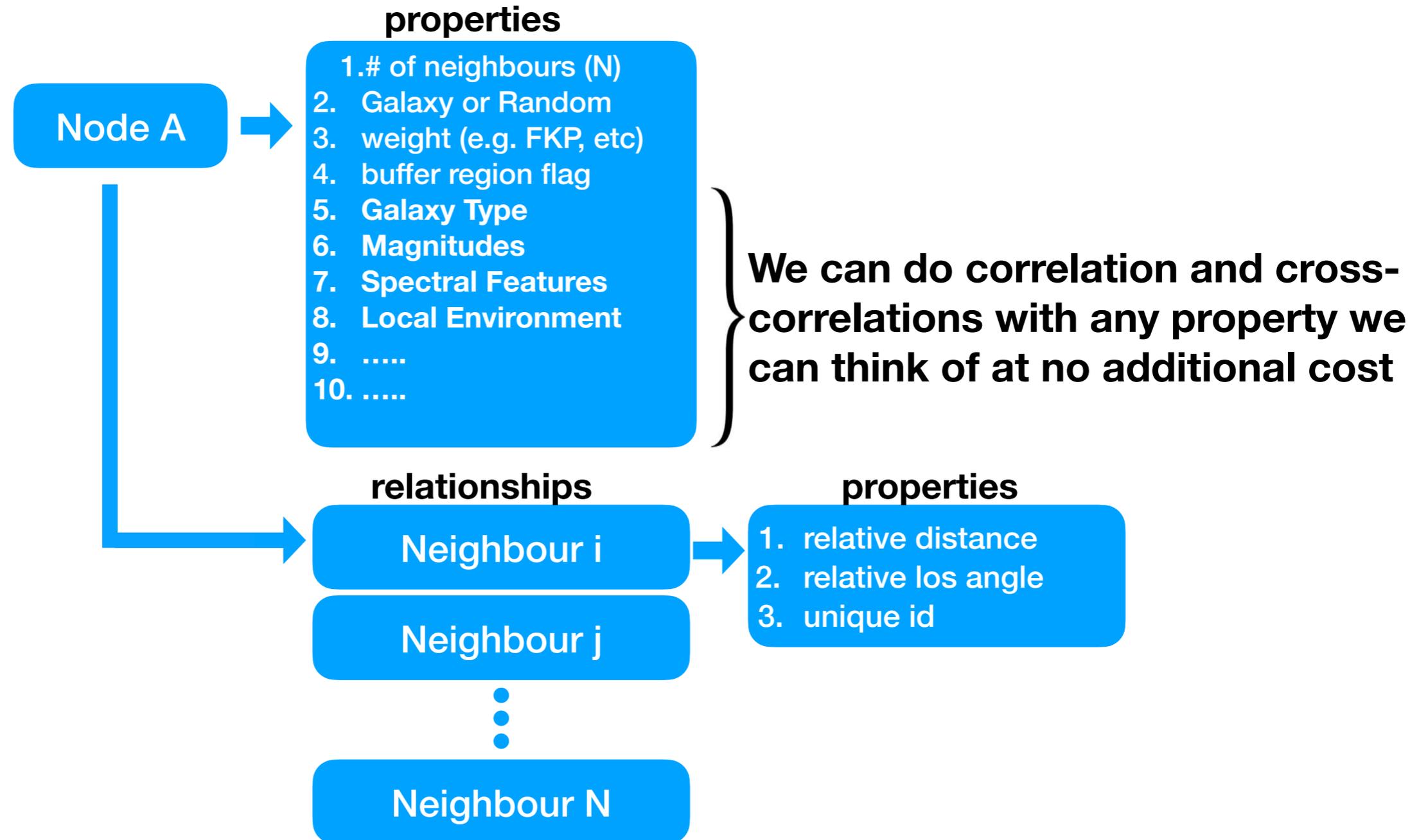
# Graph Database for exploring new quantities in galaxy evolution, cosmology

## Graph Database Structure



# Graph Database for exploring new quantities in galaxy evolution, cosmology

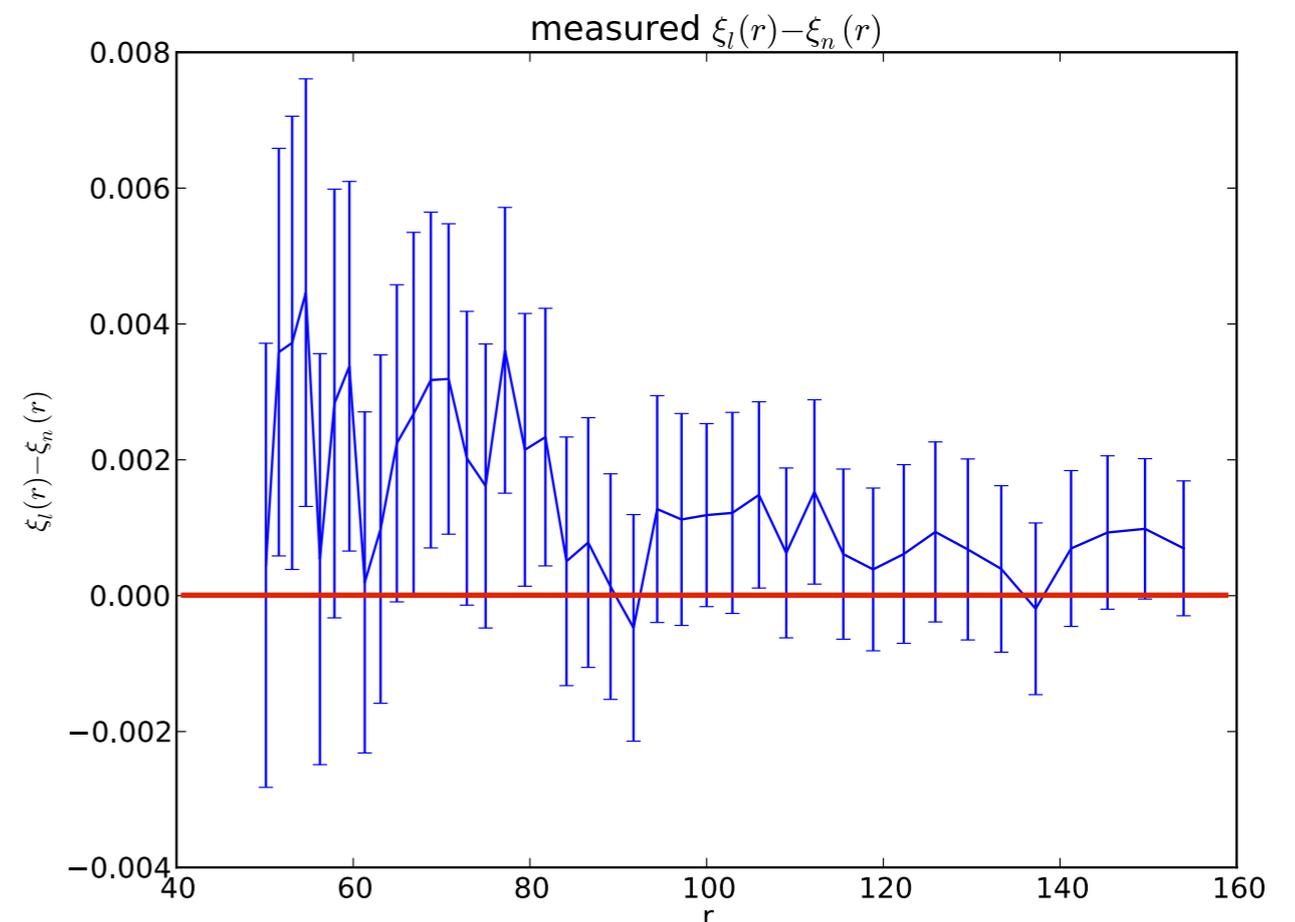
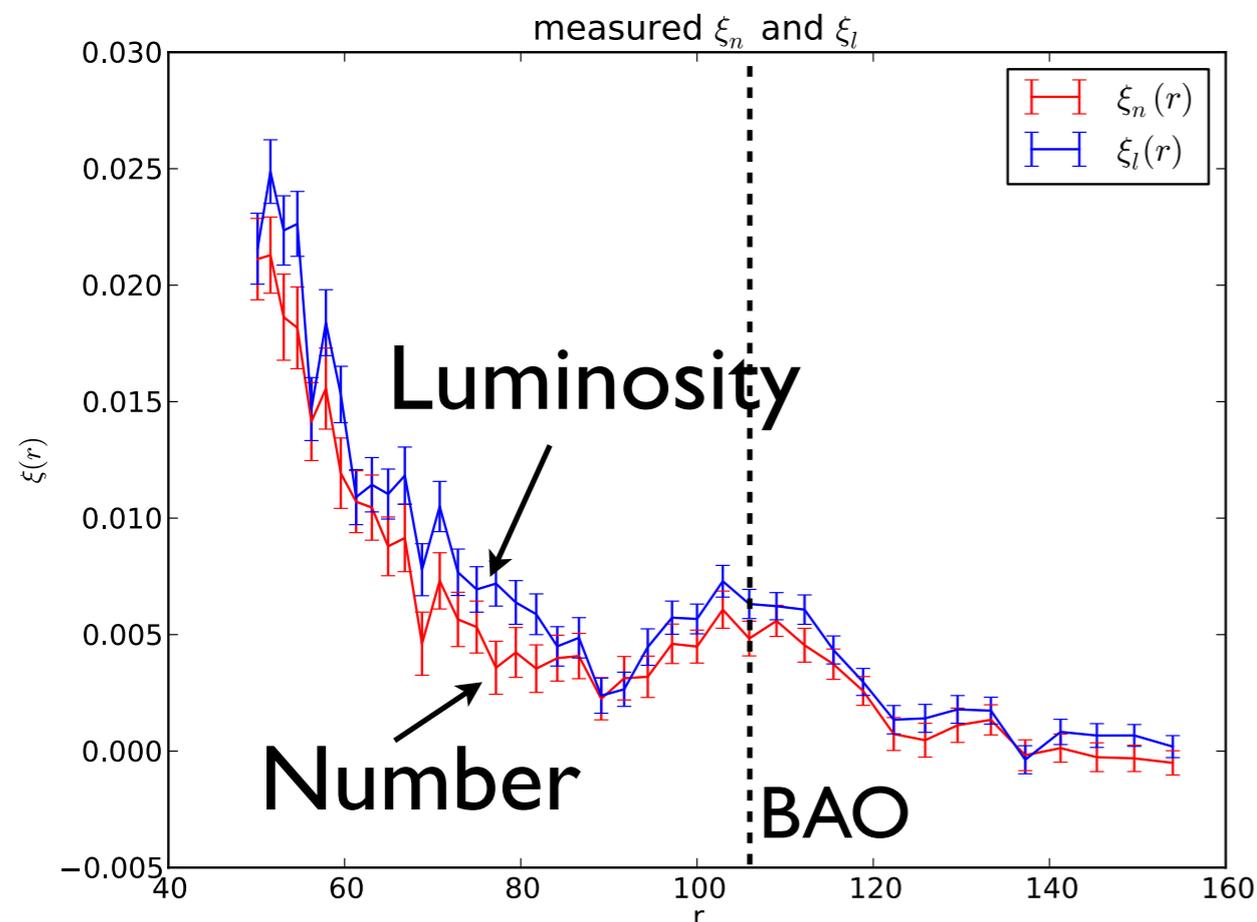
## Graph Database Structure



# Graph Database for exploring new quantities in galaxy evolution, cosmology

**Example: lets look at counting data pairs while weighting by galaxy luminosity**

- Query the database for all relationships where  $r_{\min} < r < r_{\max}$
- Count that pair weighted by its absolute luminosity
- Compare with unclustered random points
- Compute the usual Landy-Szalay estimator for the 2pCF
- But what does it mean? What information does it contain?



# Graph Database for exploring new quantities in galaxy evolution, cosmology

Following the theoretical work of Barkana & Loeb 2010

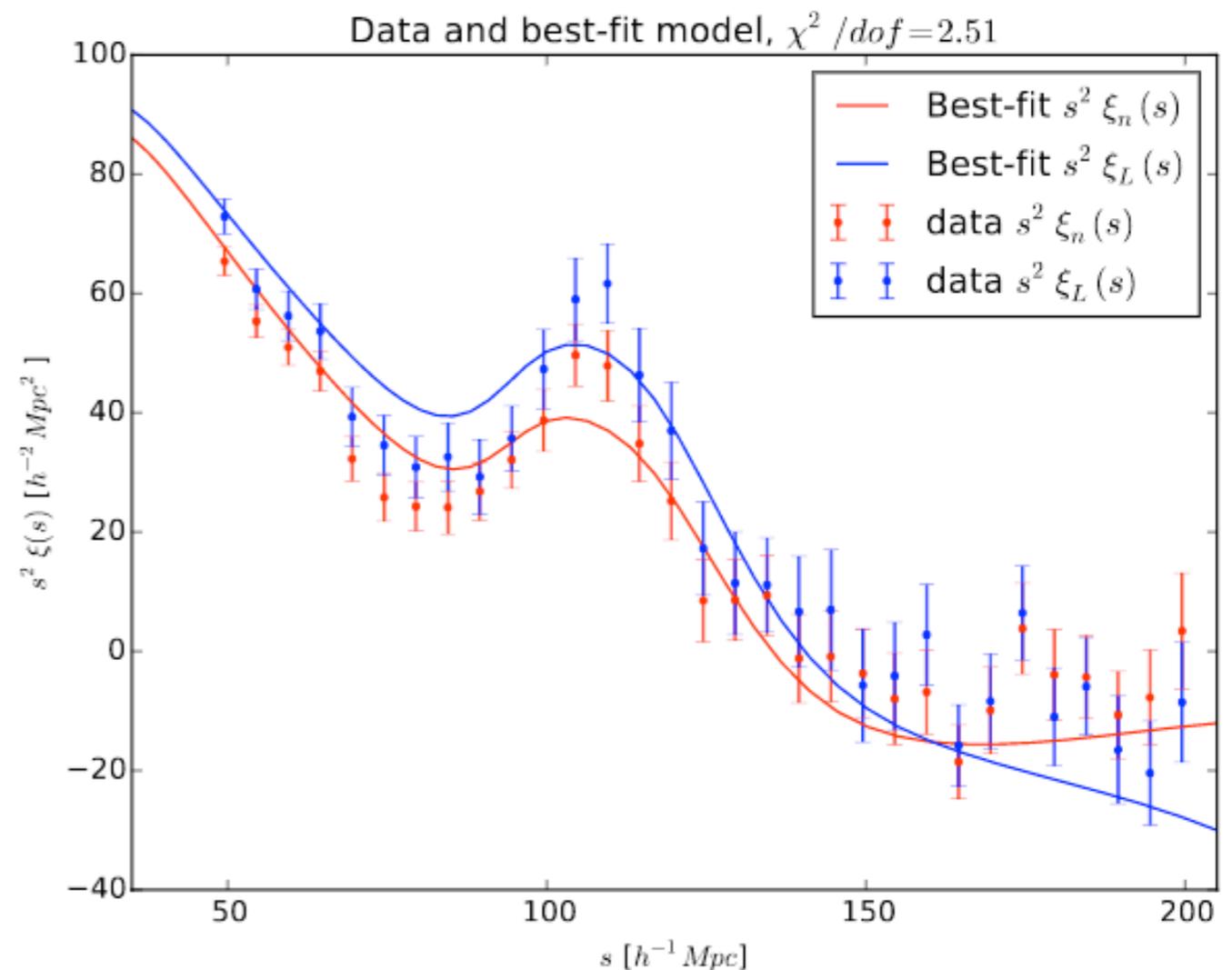
We develop a model for the luminosity weighted correlation function of galaxies:

$$\xi_L = B_{L,t}^2 \xi_{\text{tot}} + 2B_{L,t} B_{L,\Delta} \xi_{\text{add}} + B_{L,\Delta}^2 B_{\text{CIP}} \hat{\xi}_{\text{CIP}},$$

This equation has dependence on:

- A linear bias with dark matter
- large scale clustering of baryons, potentially a new quantity to consider in galaxy evolution
- Compensated Isocurvature Perturbations (CIP) between baryons and dark matter in the early universe

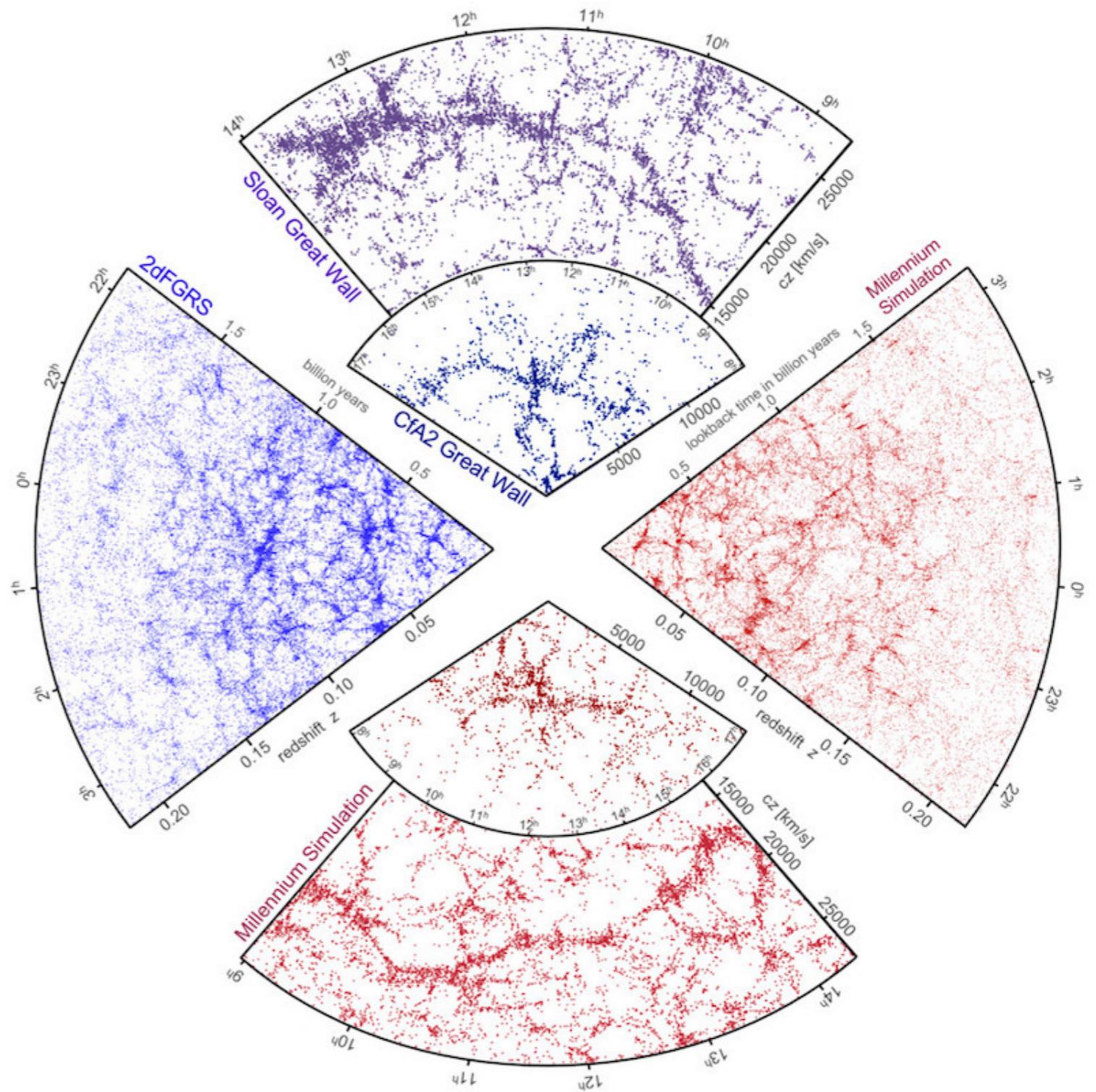
Looking at spatial cross-correlations with different quantities unlocks new physical interpretation of the data



# Machine Learning Approach

---

Use machine learning to match observation with simulation (model)



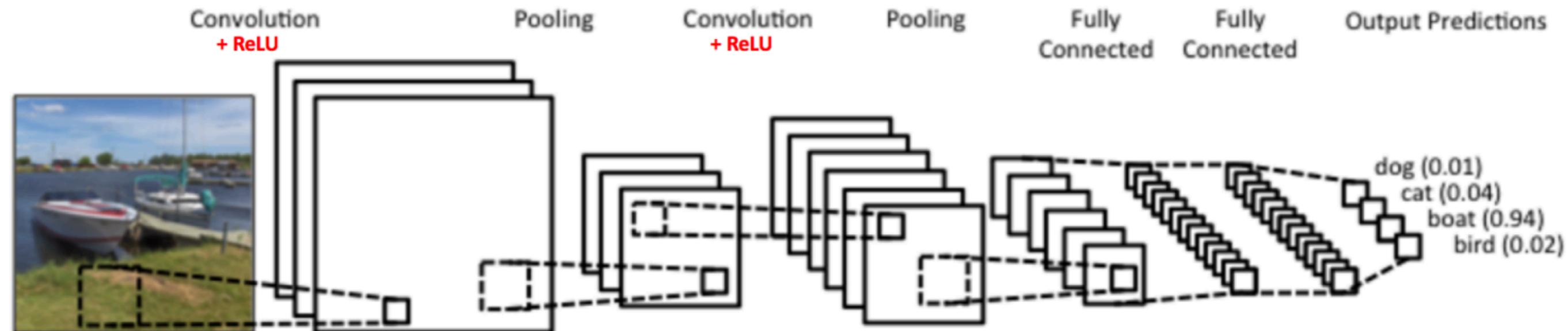
# Convolutional Neural Networks

---

A convolutional neural network for visual classification

From a number of inputs obtain a meaningful output

By training CNN on a known set of data (labelled)



We will break down each step one by one...

# Convolutional Neural Networks

---

## 1. Convolution Layer

Here are the three elements that enter into the convolution operation:

- Input image
- Feature detector
- Feature map

0	0	0	0	0	0	0
0	1	0	0	0	1	0
0	0	0	0	0	0	0
0	0	0	1	0	0	0
0	1	0	0	0	1	0
0	0	1	1	1	0	0
0	0	0	0	0	0	0

Input Image

0	0	1
1	0	0
0	1	1

Feature  
Detector

The feature detector is often referred to as a “kernel” or a “filter,” which might sound more familiar to you from other areas of physics.

# Convolutional Neural Networks

---

## Convolution Layer

Here are the three elements that enter into the convolution operation:

- Input image
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- Feature map

0	0	0	0	0	0	0
0	1	0	0	0	1	0
0	0	0	0	0	0	0
0	0	0	1	0	0	0
0	1	0	0	0	1	0
0	0	1	1	1	0	0
0	0	0	0	0	0	0

Input Image



0	0	1
1	0	0
0	1	1

Feature  
Detector



0				

Feature Map

# Convolutional Neural Networks

## Convolution Layer

Here are the three elements that enter into the convolution operation:

- Input image
- Feature detector
- Feature map

0	0	0	0	0	0	0
0	1	0	0	0	1	0
0	0	0	0	0	0	0
0	0	0	1	0	0	0
0	1	0	0	0	1	0
0	0	1	1	1	0	0
0	0	0	0	0	0	0

Input Image



0	0	1
1	0	0
0	1	1

Feature  
Detector



0	1	0	0	0
0	1	1	1	0
1	0	1	2	1
1	4	2	1	0
0	0	1	2	1

Feature Map

# Convolutional Neural Networks

## Convolution Layer

Here are the three elements that enter into the convolution operation:

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- Feature map

0	0	0	0	0	0	0
0	1	0	0	0	1	0
0	0	0	0	0	0	0
0	0	0	1	0	0	0
0	1	0	0	0	1	0
0	0	1	1	1	0	0
0	0	0	0	0	0	0

Input Image



0	0	1
1	0	0
0	1	1

Feature  
Detector



0	1	0	0	0
0	1	1	1	0
1	0	1	2	1
1	4	2	1	0
0	0	1	2	1

Feature Map

# Convolutional Neural Networks

## Convolution Layer

Here are the three elements that enter into the convolution operation:

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0	0	0	0	0	0	0
0	1	0	0	0	1	0
0	0	0	0	0	0	0
0	0	0	1	0	0	0
0	1	0	0	0	1	0
0	0	1	1	1	0	0
0	0	0	0	0	0	0

Input Image



0	0	1
1	0	0
0	1	1

Feature  
Detector



0	1	0	0	0
0	1	1	1	0
1	0	1	2	1
1	4	2	1	0
0	0	1	2	1

Feature Map

# Convolutional Neural Networks

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Here are the three elements that enter into the convolution operation:

- Input image
- Feature detector
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0	0	0	0	0	0	0
0	1	0	0	0	1	0
0	0	0	0	0	0	0
0	0	0	1	0	0	0
0	1	0	0	0	1	0
0	0	1	1	1	0	0
0	0	0	0	0	0	0

Input Image



0	0	1
1	0	0
0	1	1

Feature  
Detector



0	1	0	0	0
0	1	1	1	0
1	0	1	2	1
1	4	2	1	0
0	0	1	2	1

Feature Map

# Convolutional Neural Networks

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- Input image
- Feature detector
- Feature map

0	0	0	0	0	0	0
0	1	0	0	0	1	0
0	0	0	0	0	0	0
0	0	0	1	0	0	0
0	1	0	0	0	1	0
0	0	1	1	1	0	0
0	0	0	0	0	0	0

Input Image



0	0	1
1	0	0
0	1	1

Feature  
Detector



0	1	0	0	0
0	1	1	1	0
1	0	1	2	1
1	4	2	1	0
0	0	1	2	1

Feature Map

# Convolutional Neural Networks

## Convolution Layer

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- Input image
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- Feature map

0	0	0	0	0	0	0
0	1	0	0	0	1	0
0	0	0	0	0	0	0
0	0	0	1	0	0	0
0	1	0	0	0	1	0
0	0	1	1	1	0	0
0	0	0	0	0	0	0

Input Image



0	0	1
1	0	0
0	1	1

Feature  
Detector



0	1	0	0	0
0	1	1	1	0
1	0	1	2	1
1	4	2	1	0
0	0	1	2	1

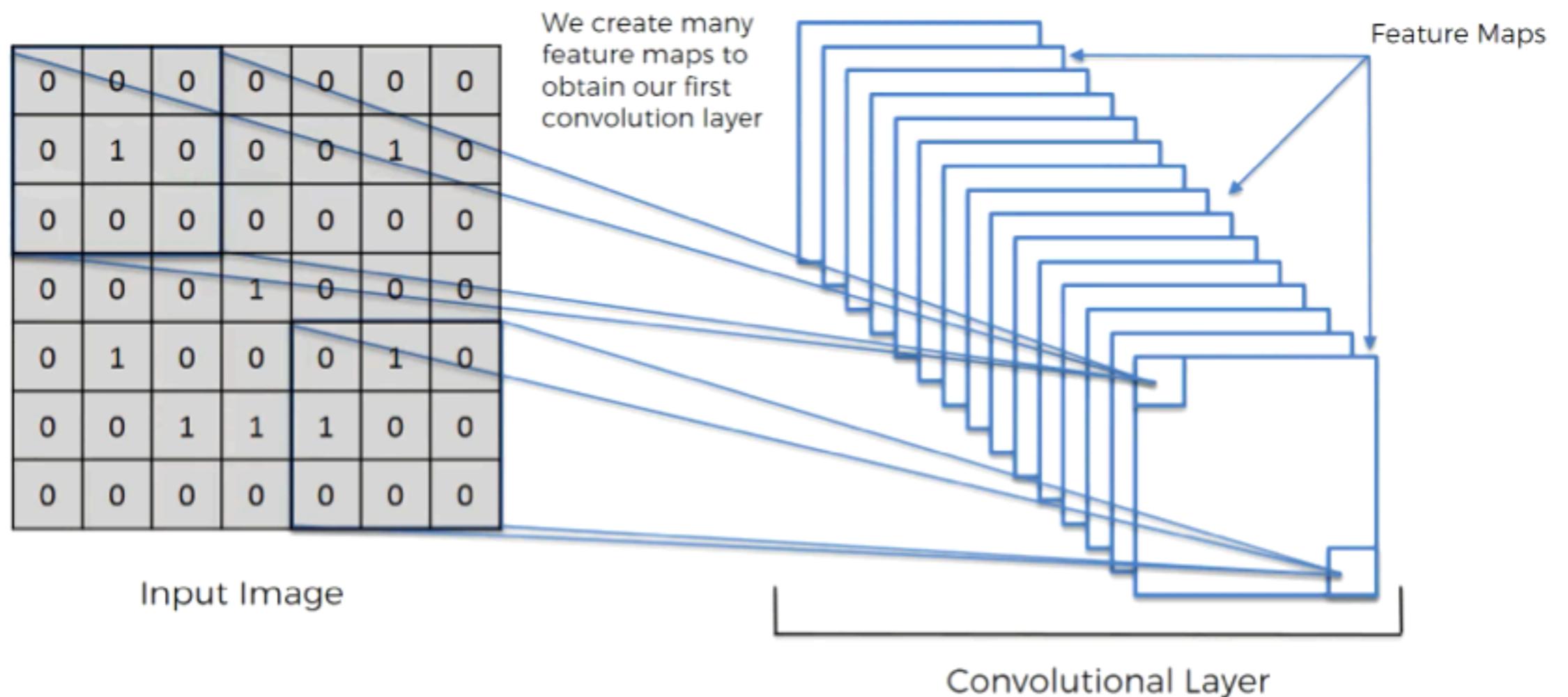
Feature Map

# Convolutional Neural Networks

## Convolution Layer

In reality, convolutional neural networks develop multiple feature detectors and use them to develop several feature maps which are referred to as convolutional layers

Through training, the network determines what features it finds important in order for it to be able to scan images and categorize them more accurately.



# Convolutional Neural Networks

---

## 1. Convolution Layer

These filters have a use in image processing and that will help give us a more intuitive feeling about them

Sharpen

0	-1	0
-1	5	-1
0	-1	0

Input image



Feature Map



# Convolutional Neural Networks

---

## 1. Convolution Layer

These filters have a use in image processing and that will help give us a more intuitive feeling about them

**Blur**

1	1	1
1	1	1
1	1	1

**Input image**



**Feature Map**



# Convolutional Neural Networks

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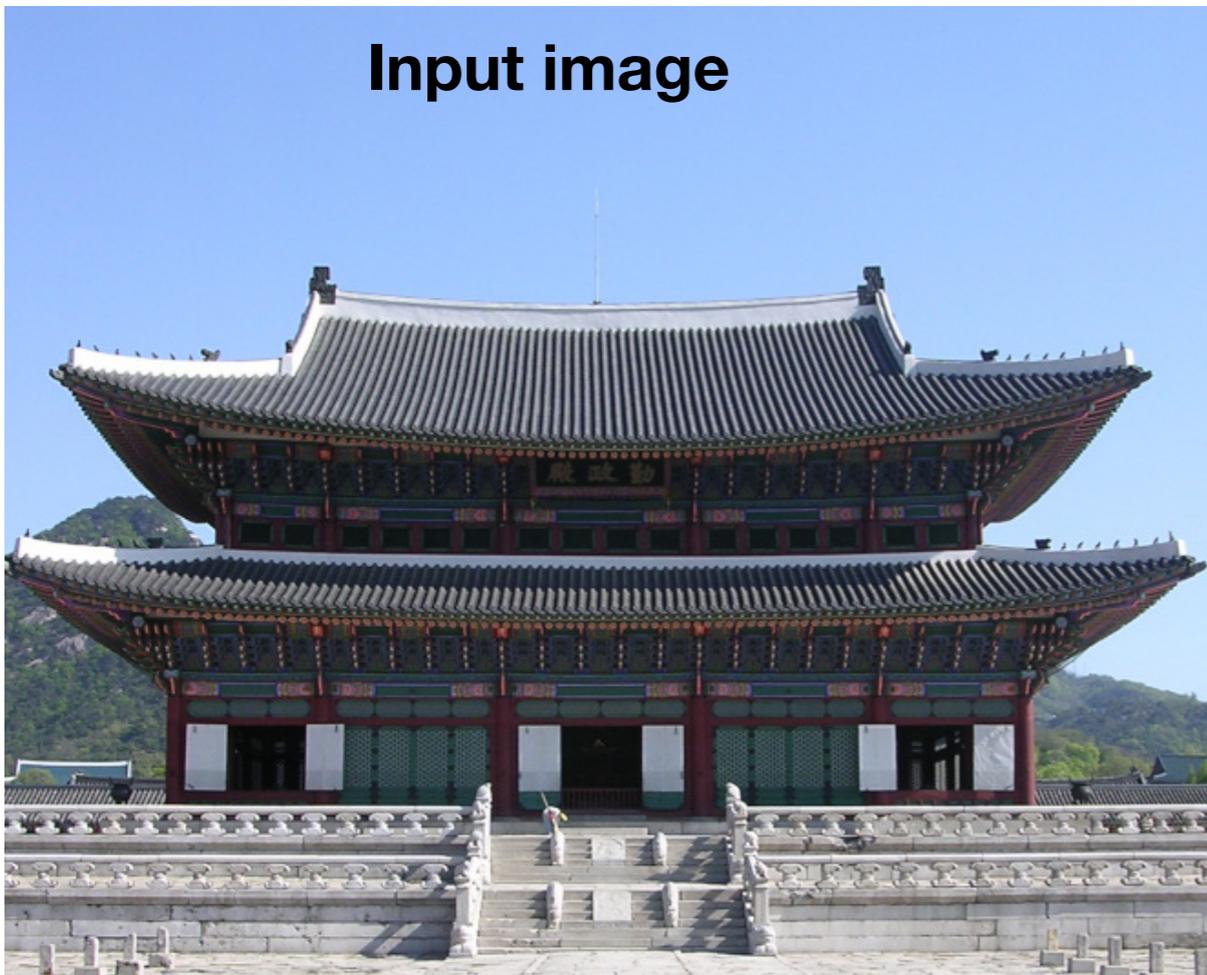
## 1. Convolution Layer

These filters have a use in image processing and that will help give us a more intuitive feeling about them

Edge Detect

0	1	0
1	-4	1
0	1	0

Input image



Feature Map

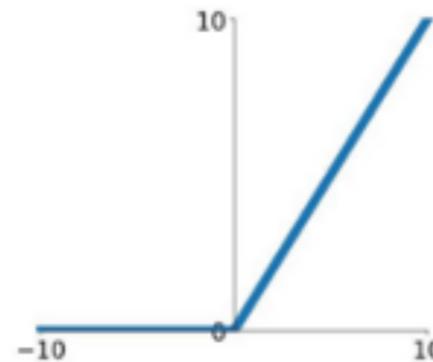


# Convolutional Neural Networks

## 2. Activation Function (eg ReLU)

Rectified Linear Unit (ReLU) is an element wise operation (applied per pixel) and replaces all negative pixel values in the feature map by zero. The purpose of ReLU is to introduce non-linearity in our ConvNet, since most of the real-world data we would want our ConvNet to learn would be non-linear

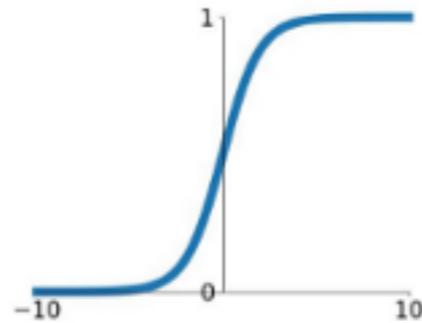
**ReLU**  
 $\max(0, x)$



Others...

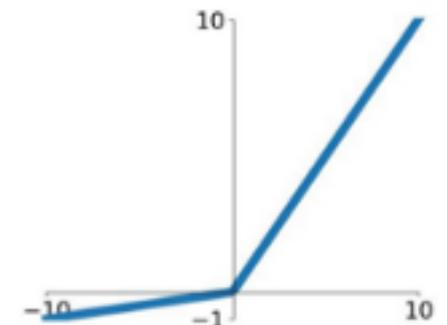
**Sigmoid**

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



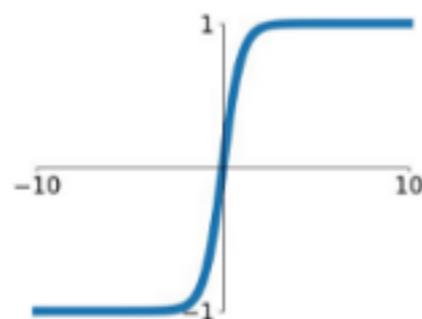
**Leaky ReLU**

$$\max(0.1x, x)$$



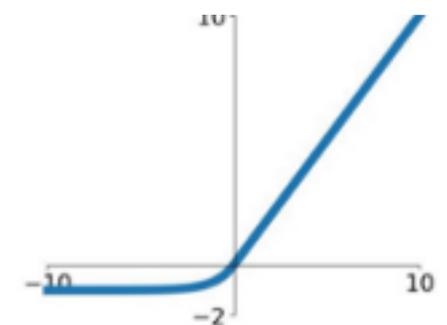
**tanh**

$$\tanh(x)$$



**ELU**

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



# Convolutional Neural Networks

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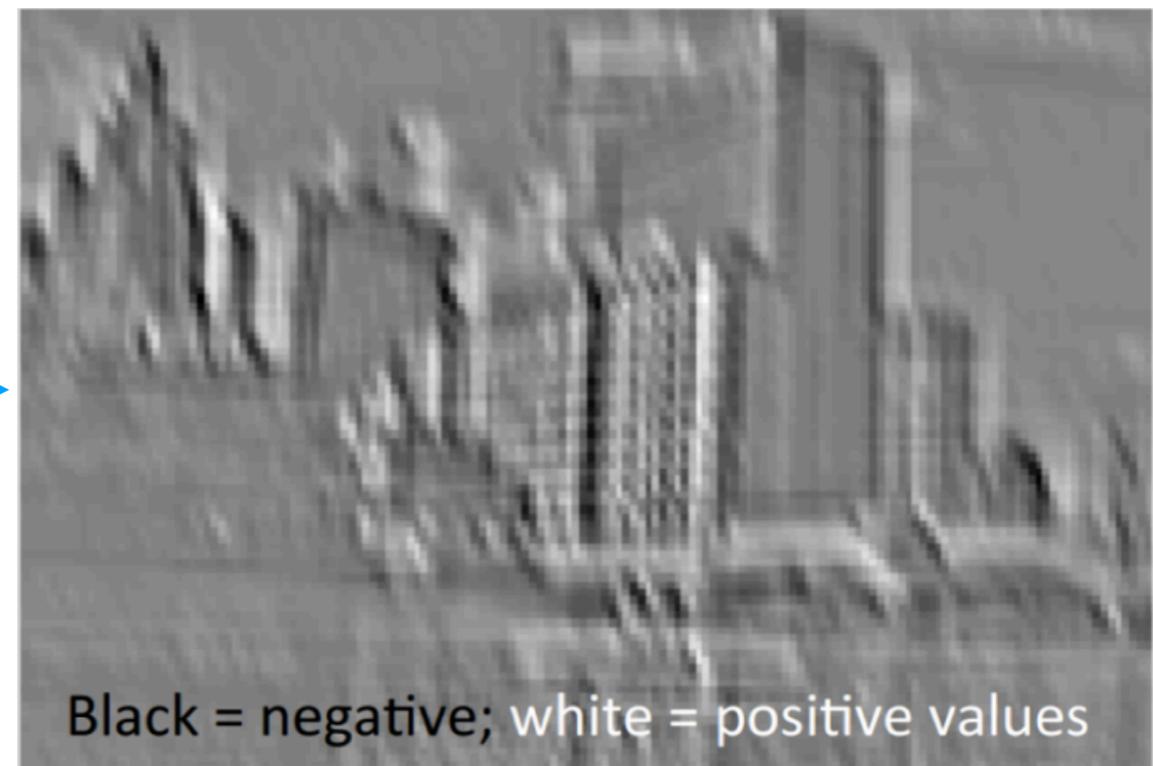
## 2. ReLU

Rectified Linear Unit (ReLU) is an element wise operation (applied per pixel) and replaces all negative pixel values in the feature map by zero. The purpose of ReLU is to introduce non-linearity in our ConvNet, since most of the real-world data we would want our ConvNet to learn would be non-linear

**Original**



**Feature detected image**



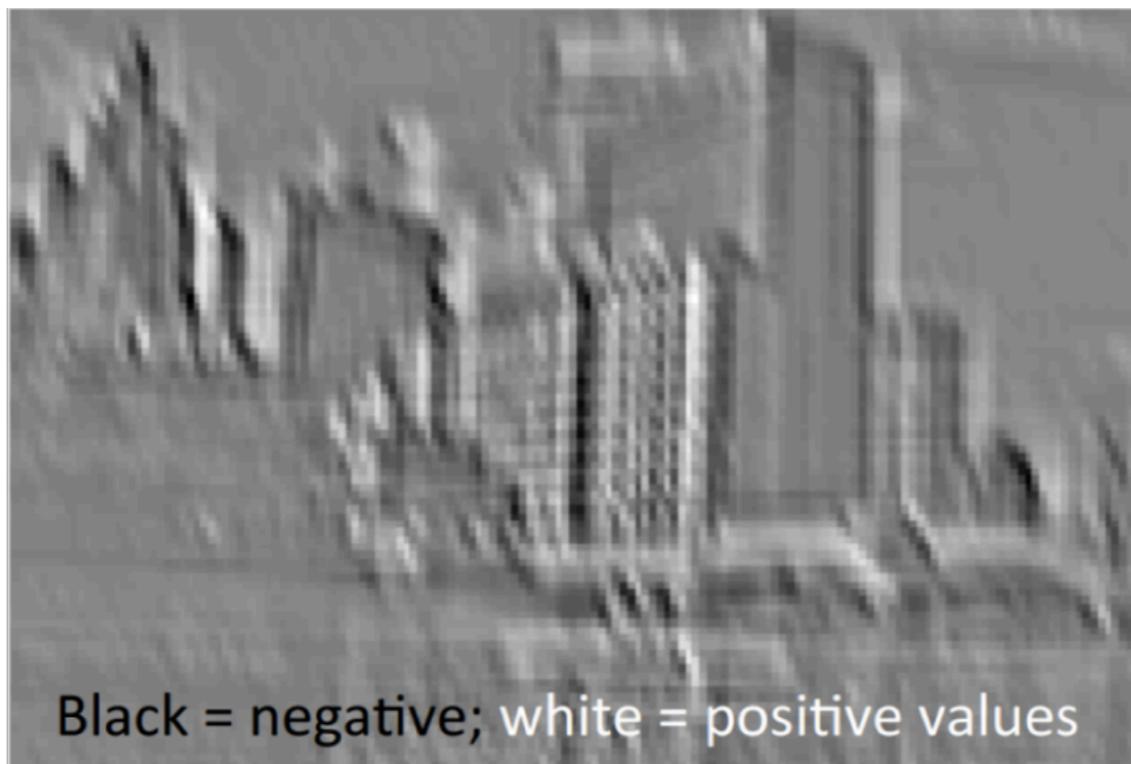
# Convolutional Neural Networks

---

## 2. ReLU

Rectified Linear Unit (ReLU) is an element wise operation (applied per pixel) and replaces all negative pixel values in the feature map by zero. The purpose of ReLU is to introduce non-linearity in our ConvNet, since most of the real-world data we would want our ConvNet to learn would be non-linear

**Feature detected image**



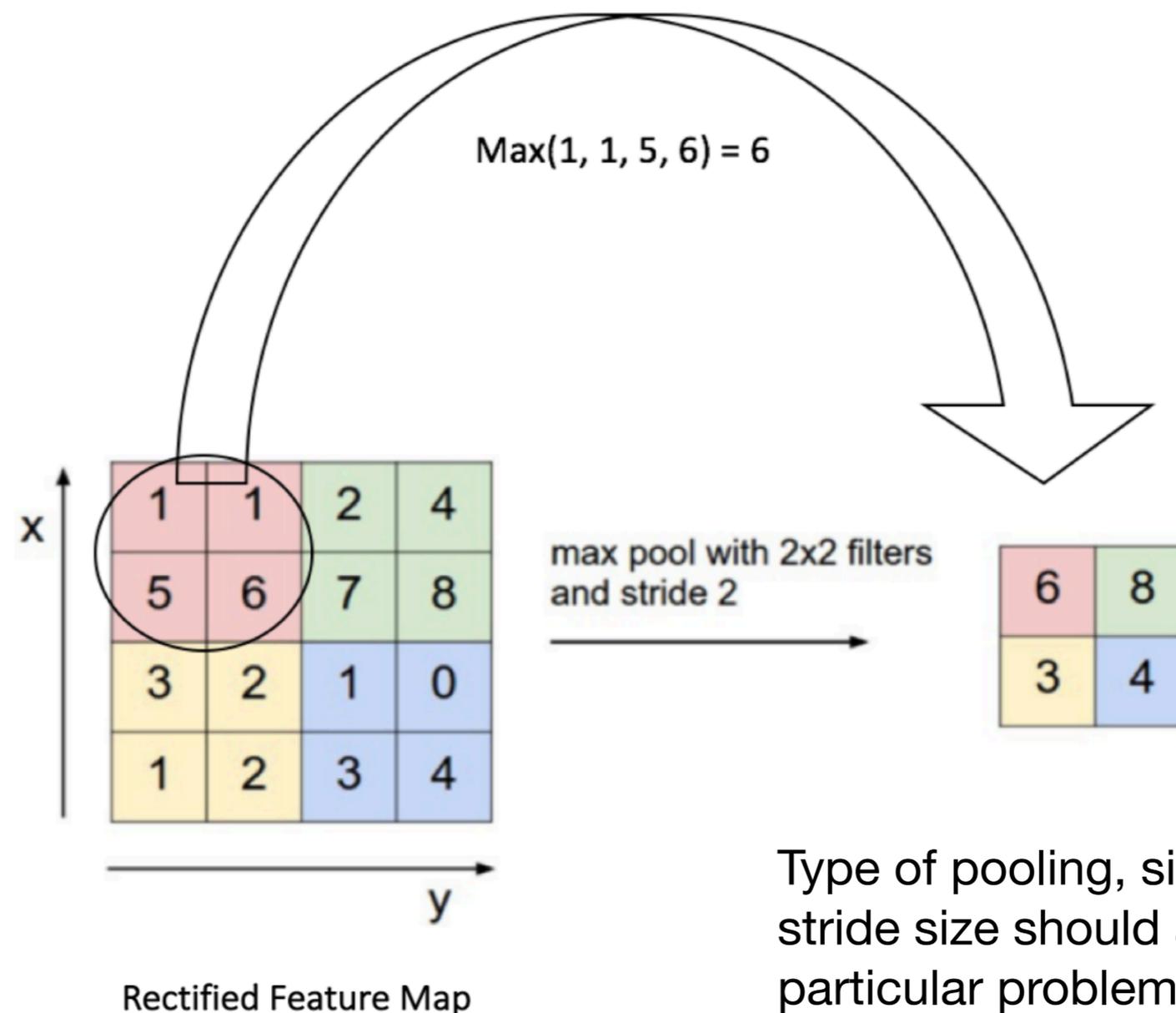
**Activated Feature Map**



# Convolutional Neural Networks

## 3. Pooling

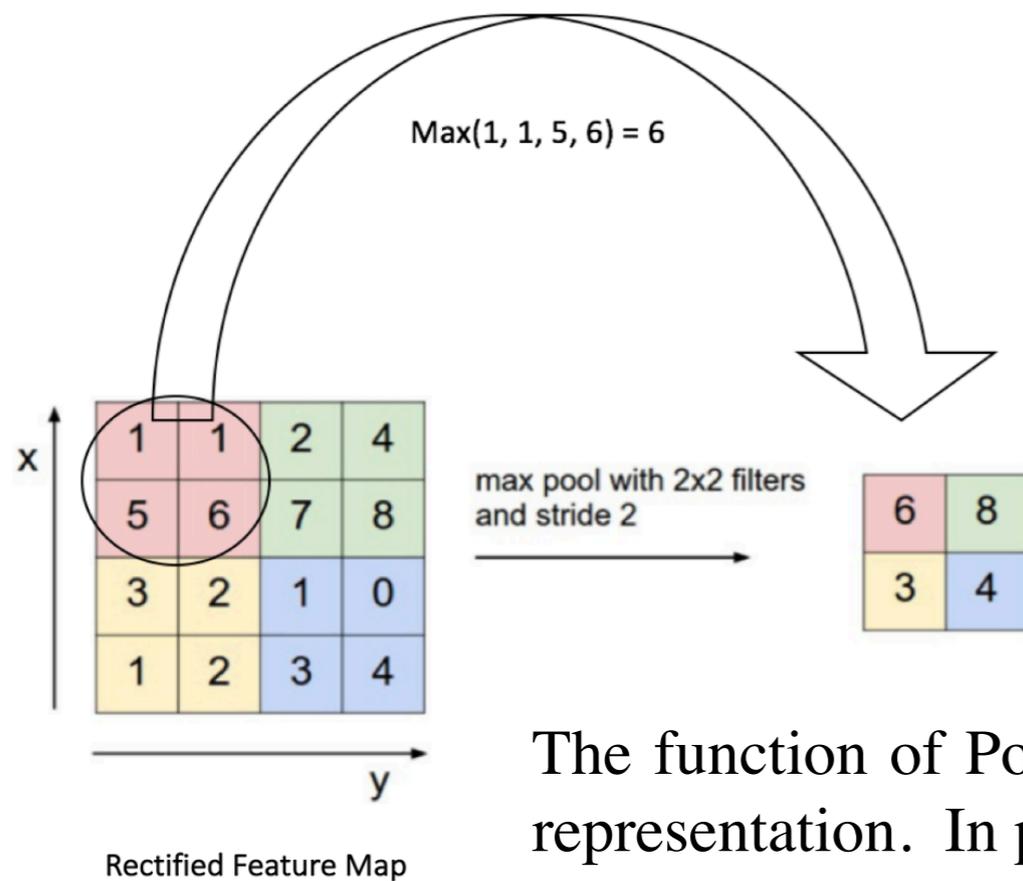
Spatial Pooling (also called subsampling or downsampling) reduces the dimensionality of each feature map but retains the most important information. Spatial Pooling can be of different types: Max, Average, Sum etc.



Type of pooling, size of filter window and stride size should all be tested for your particular problem

# Convolutional Neural Networks

## 3. Pooling



The function of Pooling is to progressively reduce the spatial size of the input representation. In particular, pooling

- makes the input representations (feature dimension) smaller and more manageable
- reduces the number of parameters and computations in the network, therefore, controlling overfitting
- makes the network invariant to small transformations, distortions and translations in the input image.
- helps us arrive at an almost scale invariant representation of our image (the exact term is “equivariant”). This is very powerful since we can detect objects in an image no matter where they are located

# Convolutional Neural Networks

---

## 4. Flatten

1	1	0
4	2	1
0	2	1

Pooled Feature Map

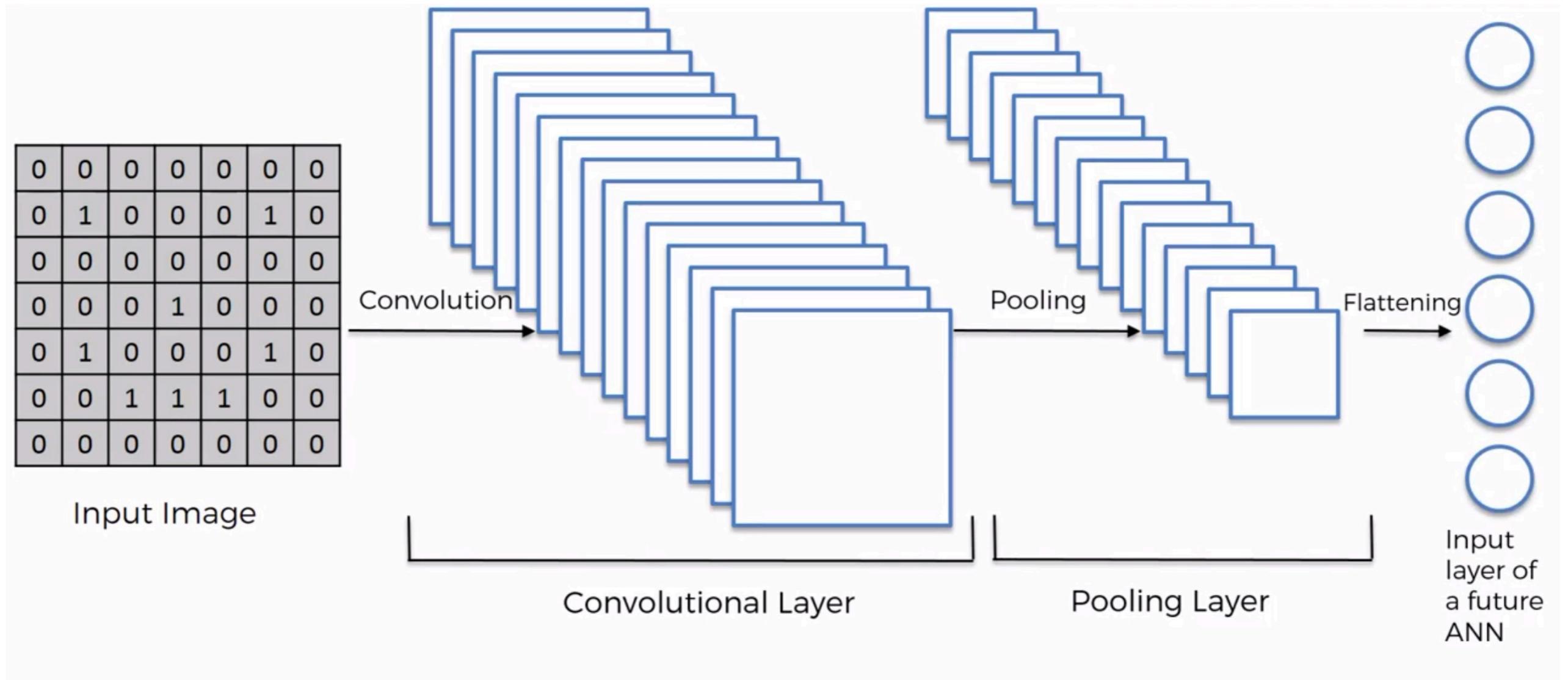
Flattening



1
1
0
4
2
1
0
2
1

# Convolutional Neural Networks

## 4. Flatten

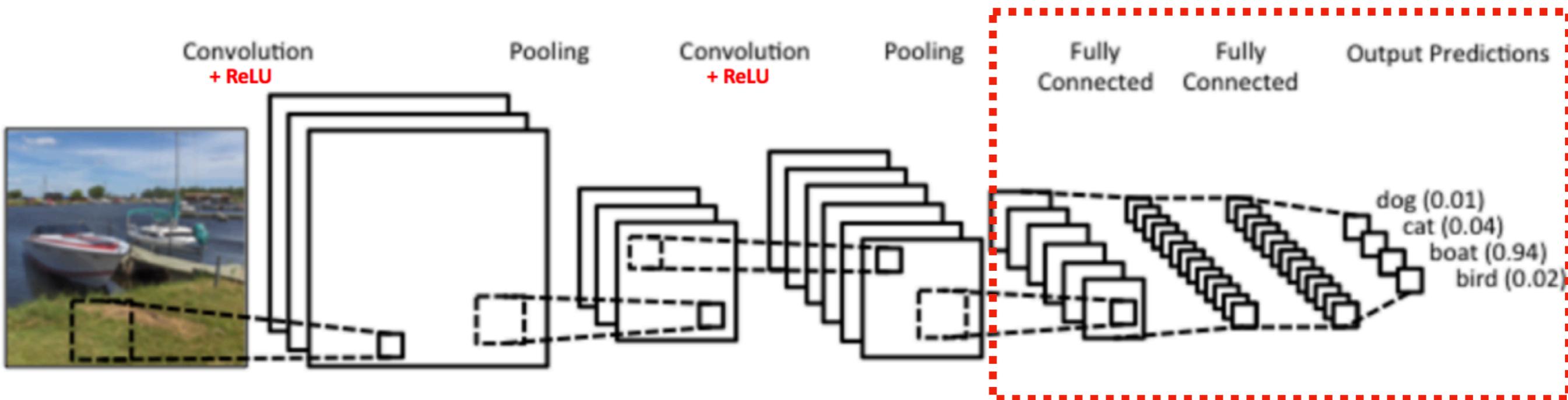


# Convolutional Neural Networks

## 5. Fully connected layer(s)

The Fully Connected layer is a traditional Multi Layer Network that uses a softmax activation function in the output layer. The term “Fully Connected” implies that every neuron in the previous layer is connected to every neuron on the next layer.

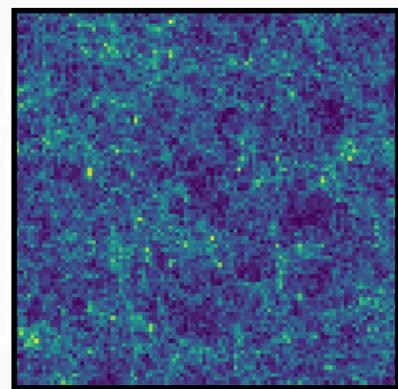
The output from the convolutional and pooling layers represent high-level features of the input image. The purpose of the Fully Connected layer is to use these features for classifying the input image into various classes based on the training dataset.



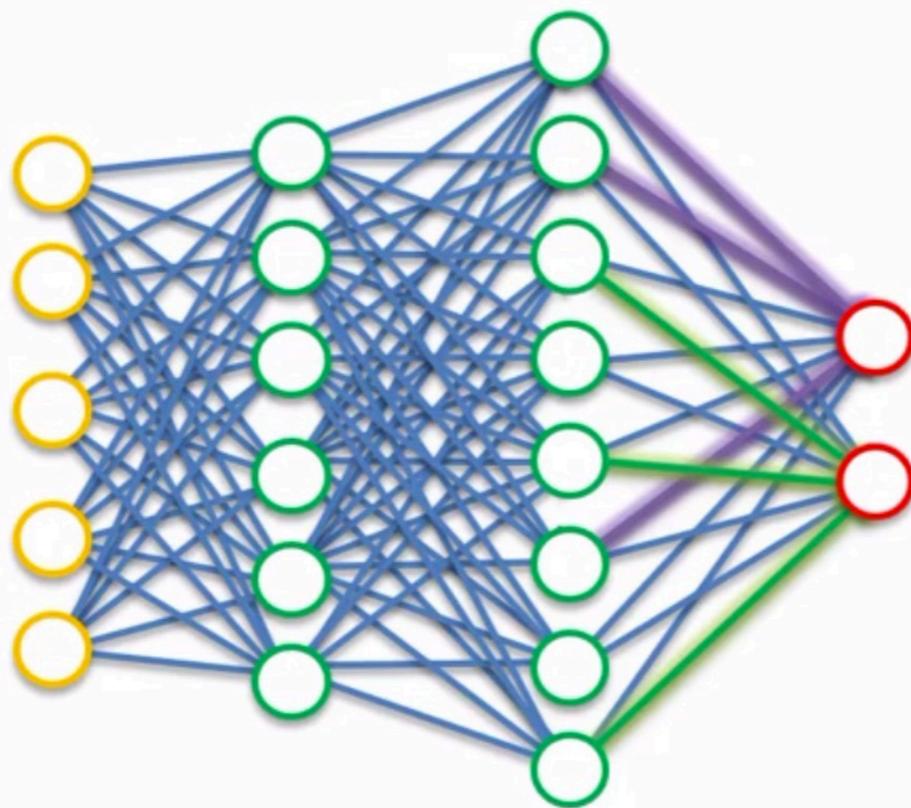
# Convolutional Neural Networks

---

## 5. Fully connected layer(s)



.....  
Flattening →



**Cosmological parameters  
Or  
Cosmological Models**

**A Standard Multi Layer Neural Network**

# Deep Learning the Large Scale Structure

---

**Ok lets apply this to cosmology!**

# Deep Learning the Large Scale Structure

Ravanbakhsh et al. (2017), Mathuriya et al. (2018) showed that convolutional neural networks can be trained to predict cosmological parameters from the visual shape of the large scale structure, i.e. the filaments, clusters and voids of the cosmic density field.

500 COmoving Lagrangian Acceleration(COLA) simulations

512Mpc box with  $512^3$  dark matter particles

Output at  $z=0$

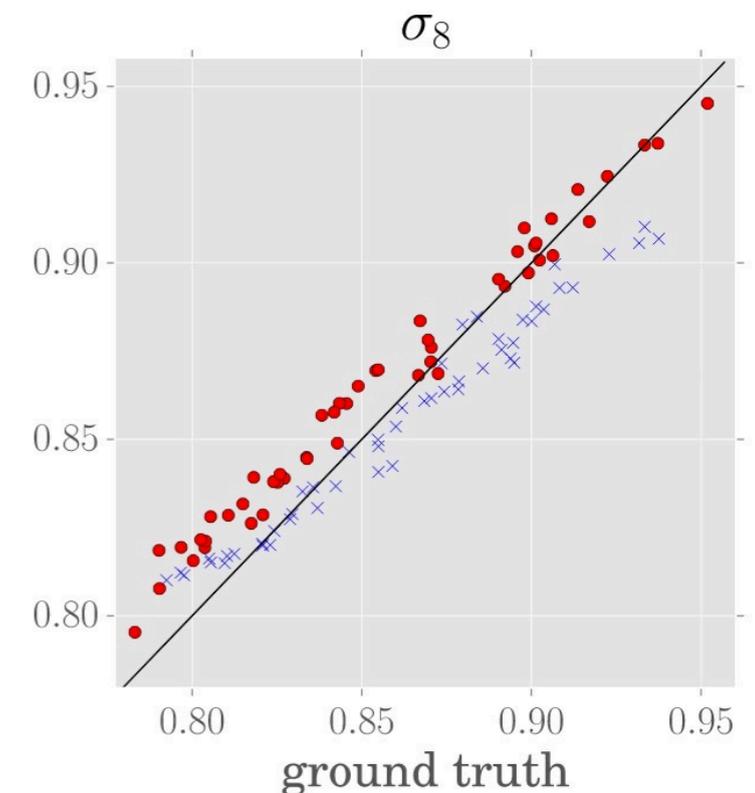
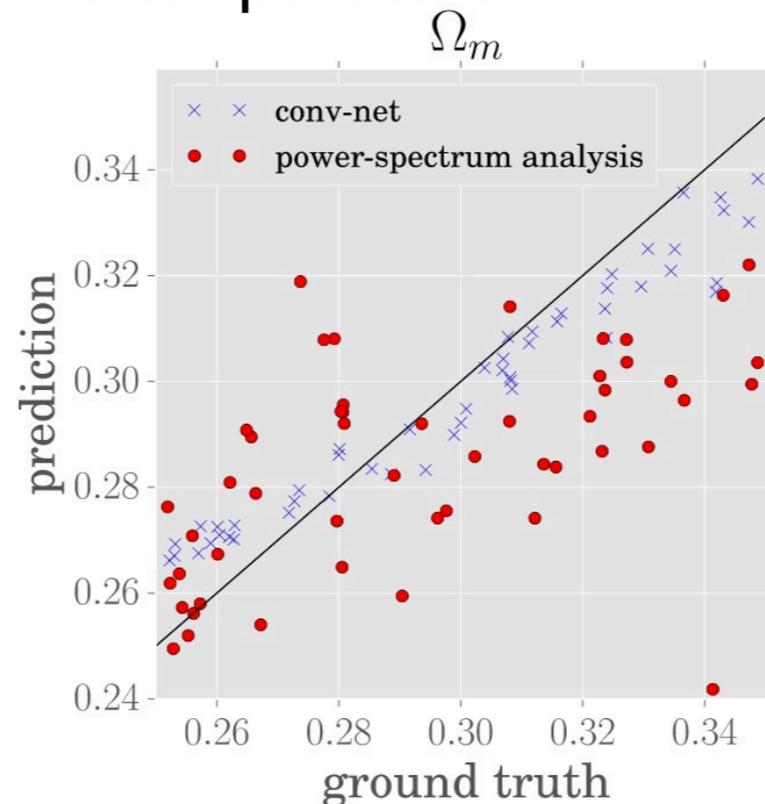
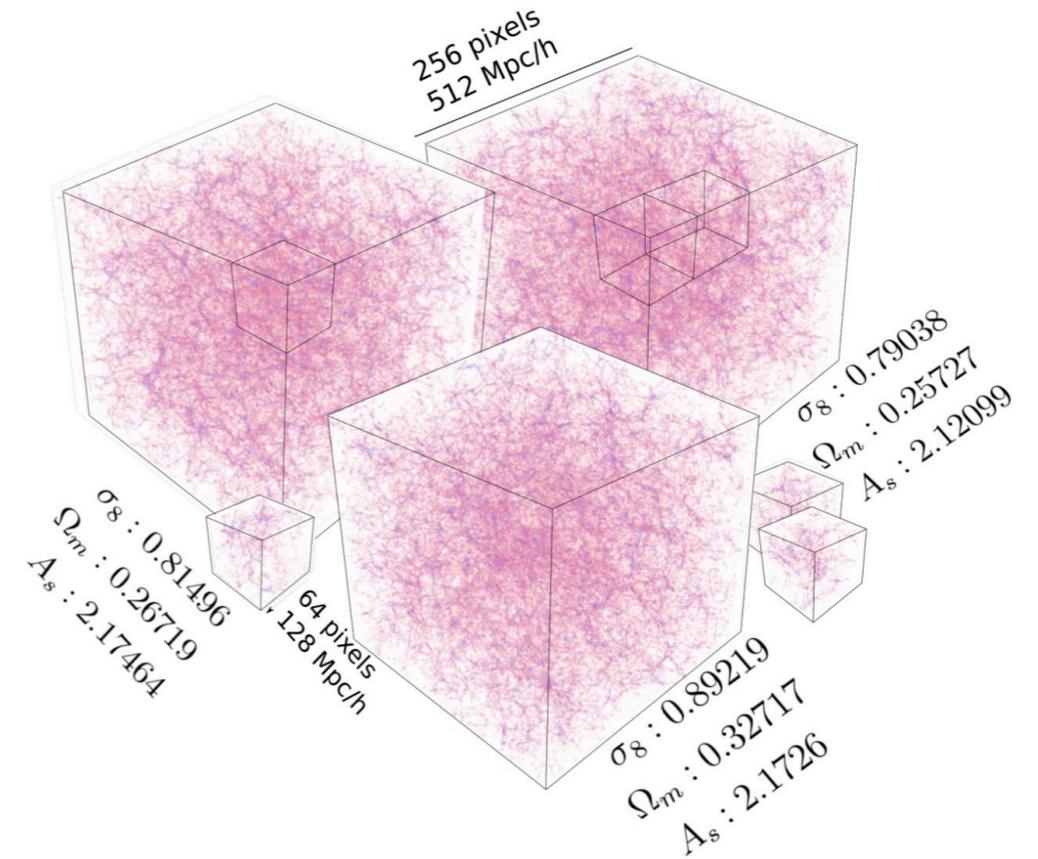
**Limitations:**

**Cubic volume at  $z=0$**

**Real space**

**Dark Matter particles**

**Fixed Architecture**



# Deep Learning the Large Scale Structure

In a grid of 31x15  
parameter combinations

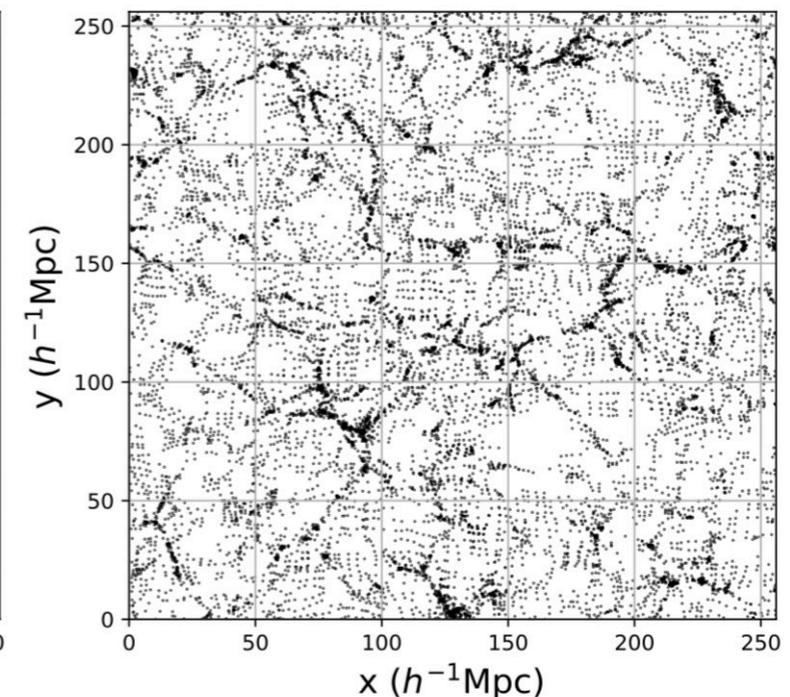
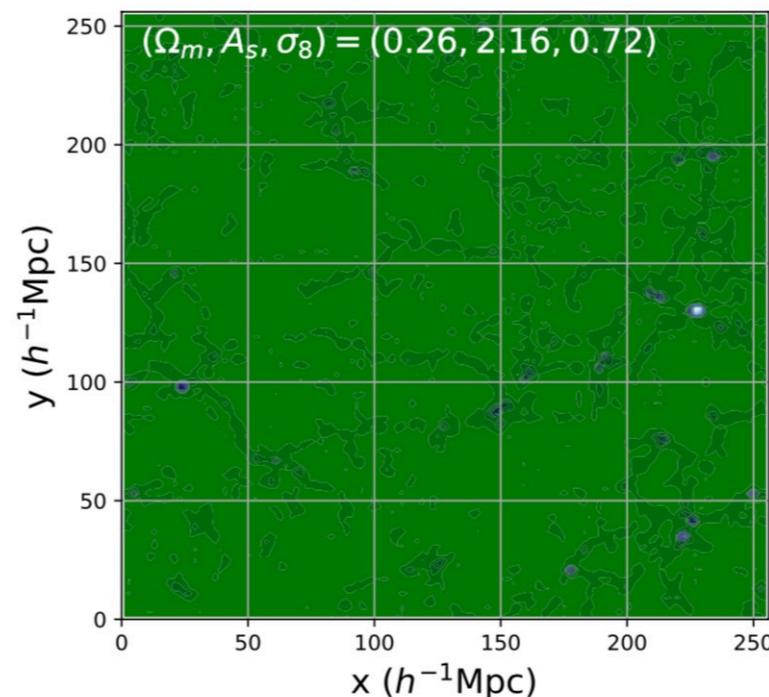
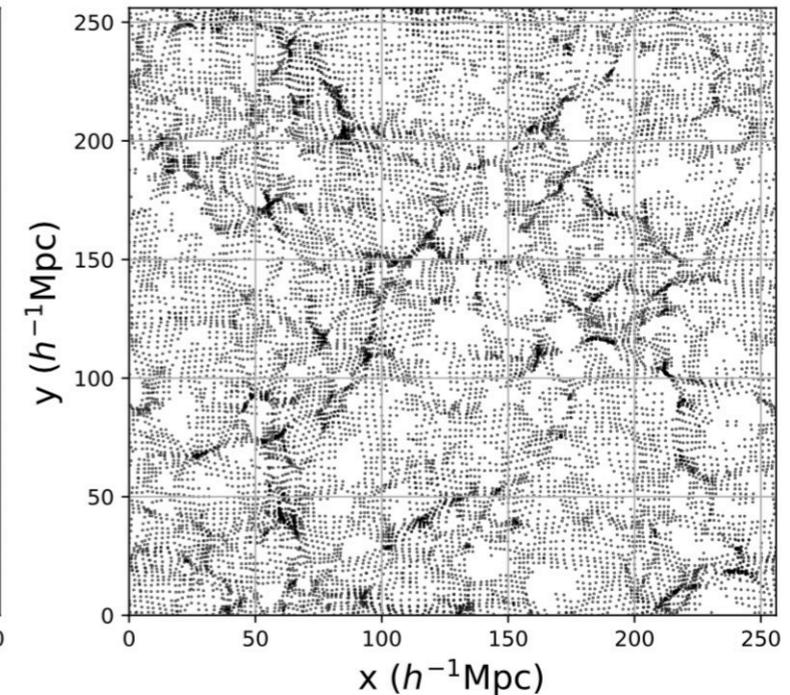
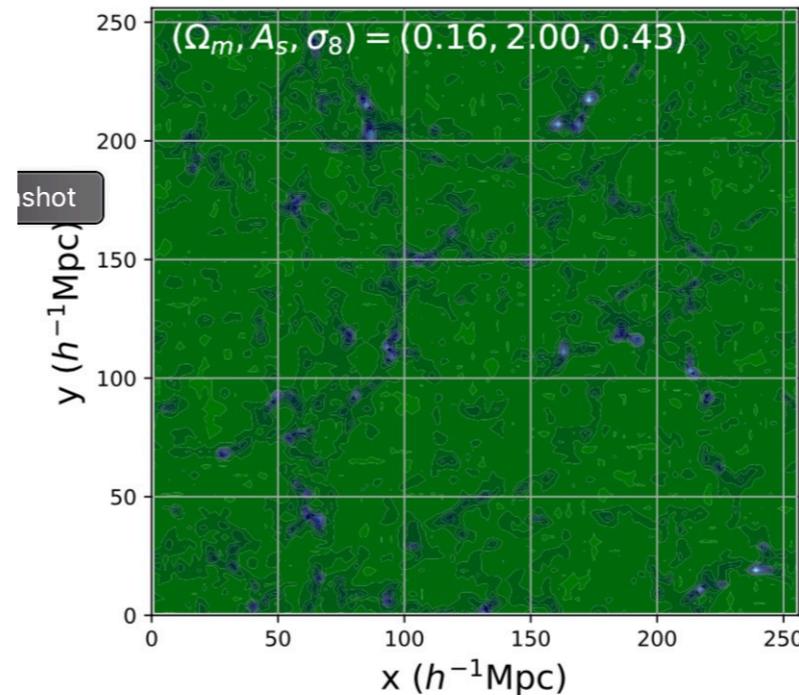
$$0.16 < \Omega_M < 0.46$$

$$0.4 < \sigma_8 < 1.1$$

We run COLA DM simulations with  
with  $128^3$  particles, in a 256 Mpc  
box, using timesteps 40 output at  $z=0$ .

We grid the data onto 2Mpc voxels.

The input of the whole network is a  
 $32^3$ -voxel (i.e.  $(64\text{Mpc})^3$ ) subcube of  
the density field.

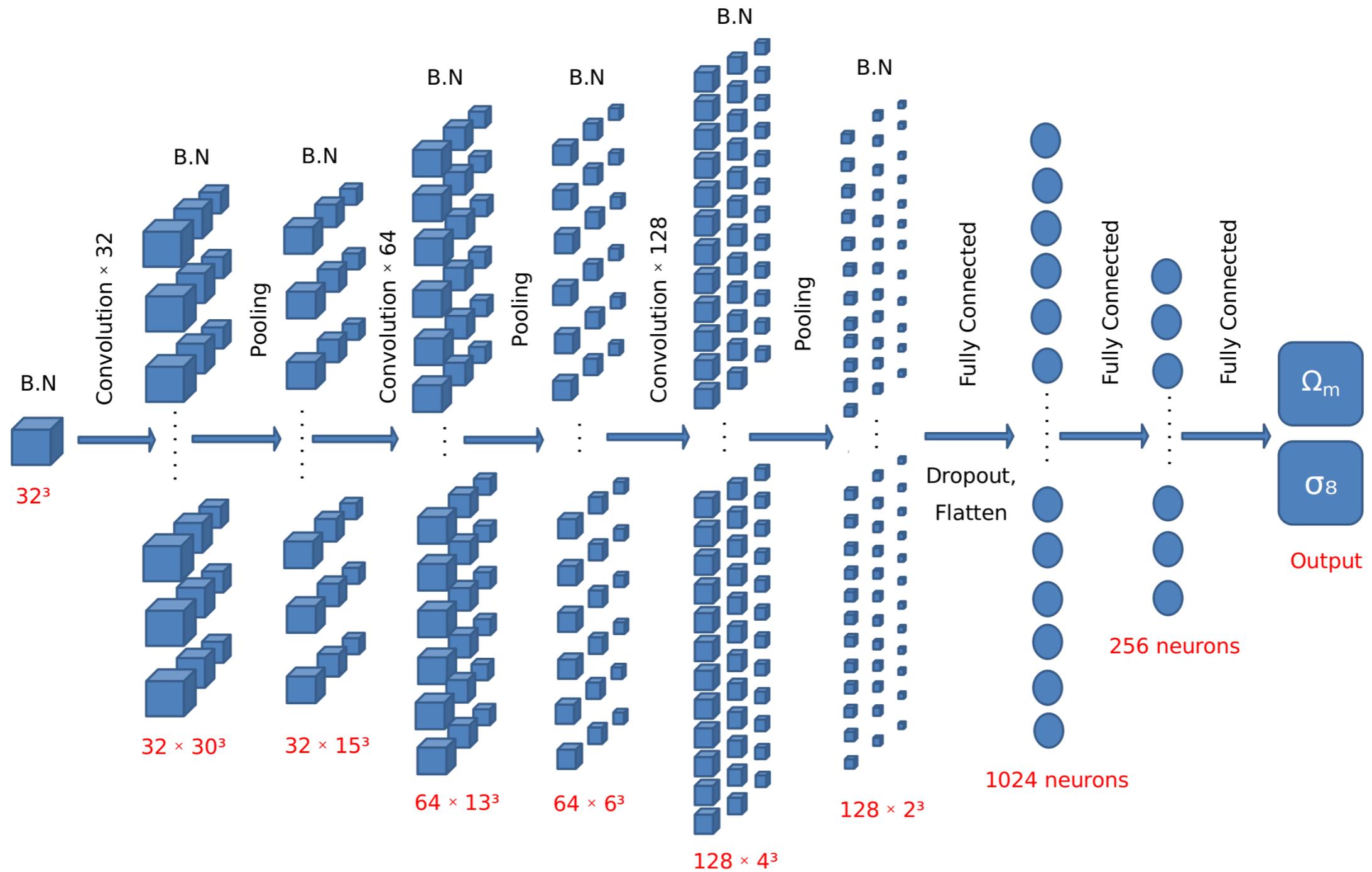


arXiv:1908.10590

Pan, Liu, Forero-Romero, Sabiu, Li, Miao, (led by) Xiao-Dong Li

# Deep Learning the Large Scale Structure

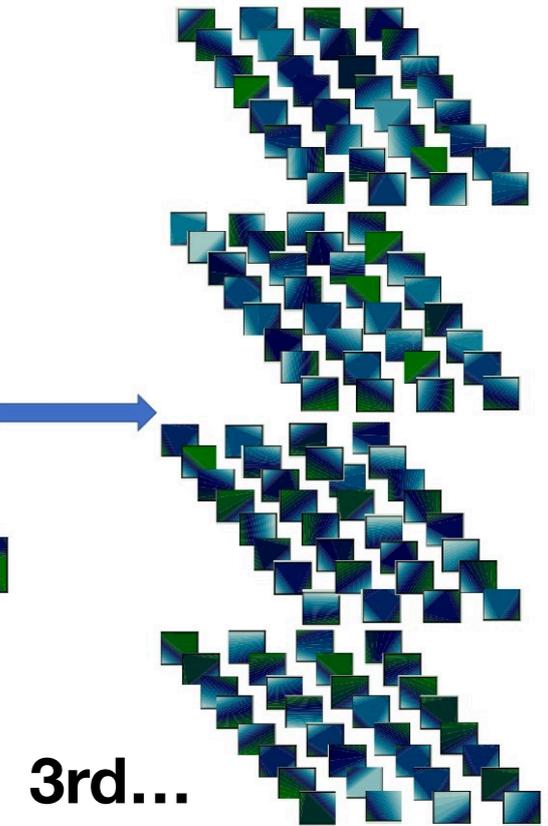
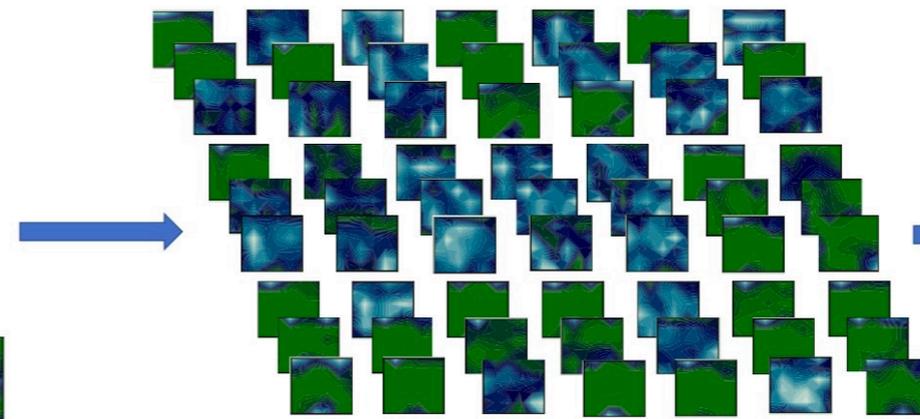
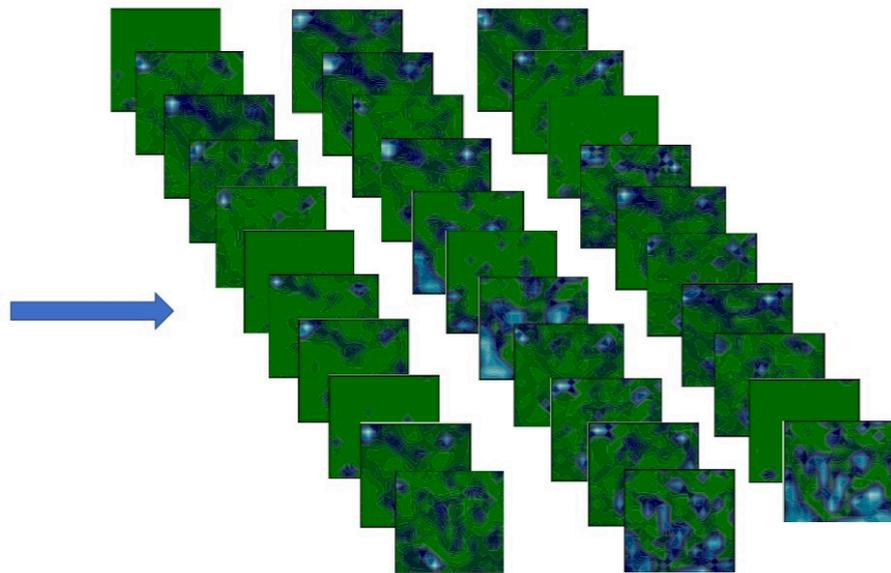
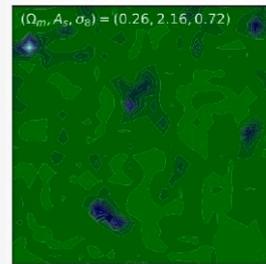
## Default Architecture



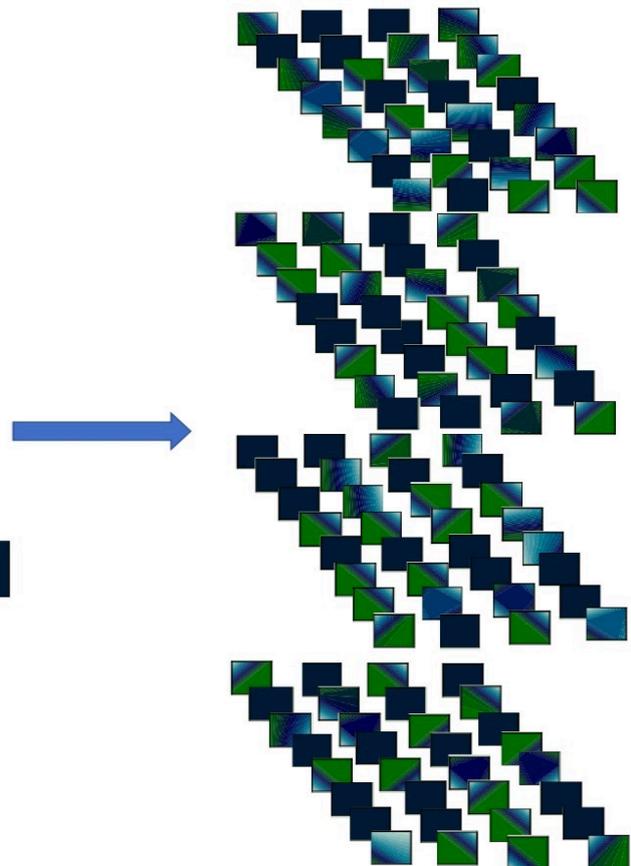
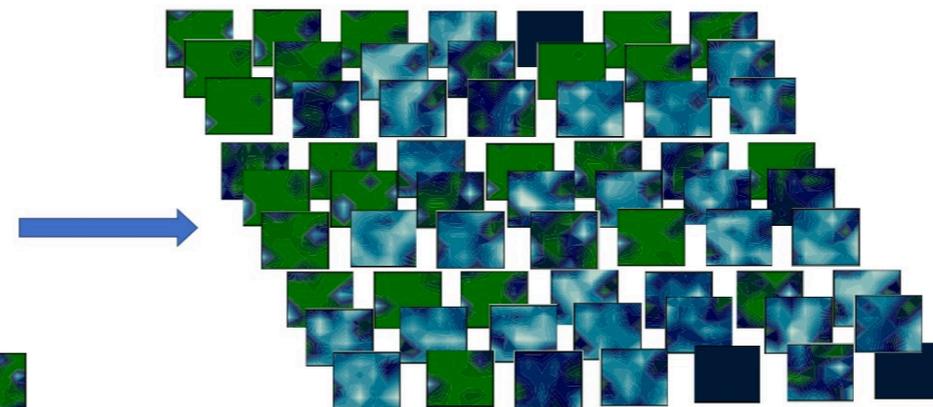
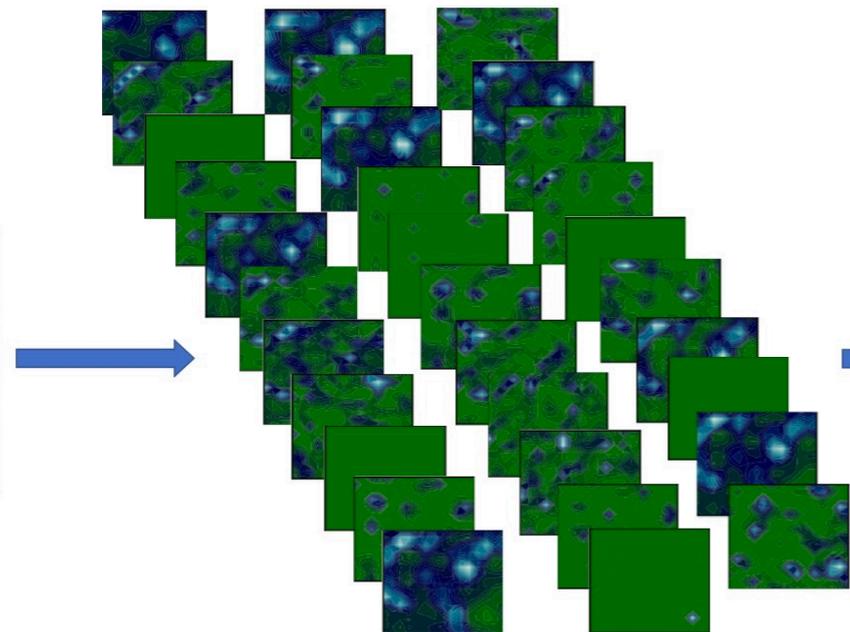
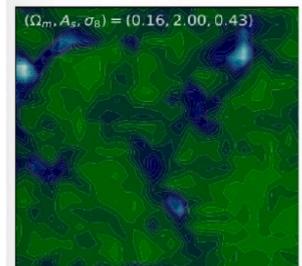
# Deep Learning the Large Scale Structure

## Inspecting the CNN

$\Omega_m = 0.26$



$\Omega_m = 0.16$



# Deep Learning the Large Scale Structure

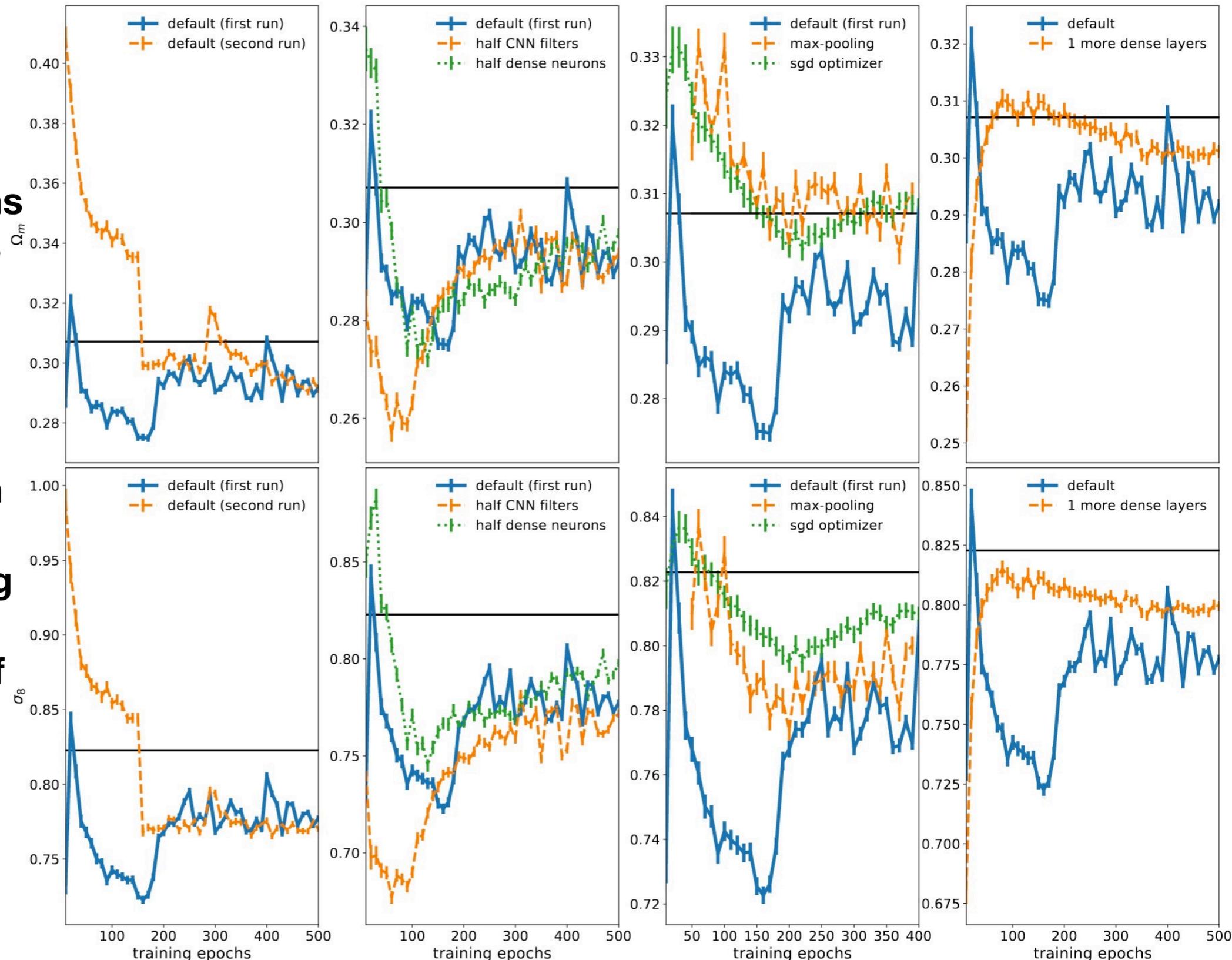
## Learning Curves

Varying:

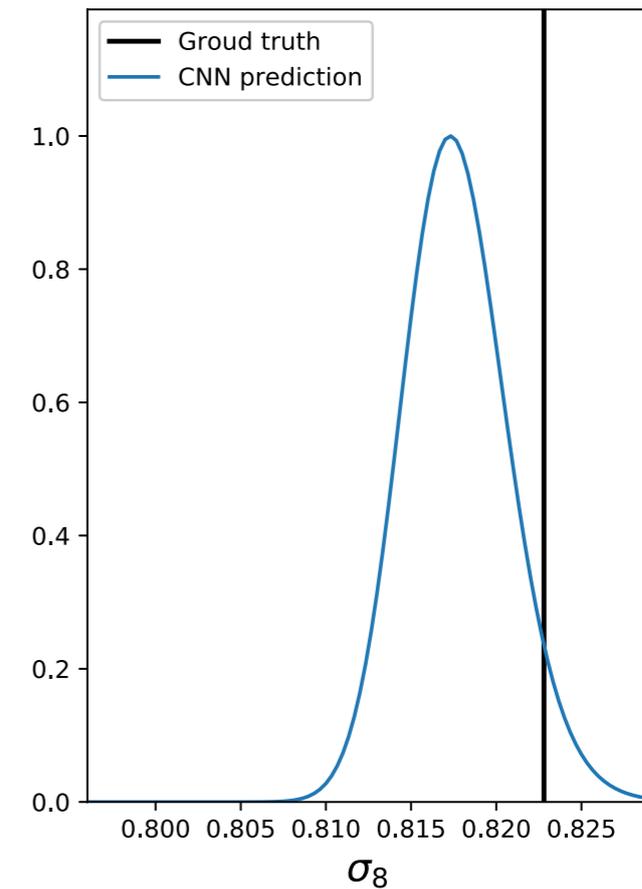
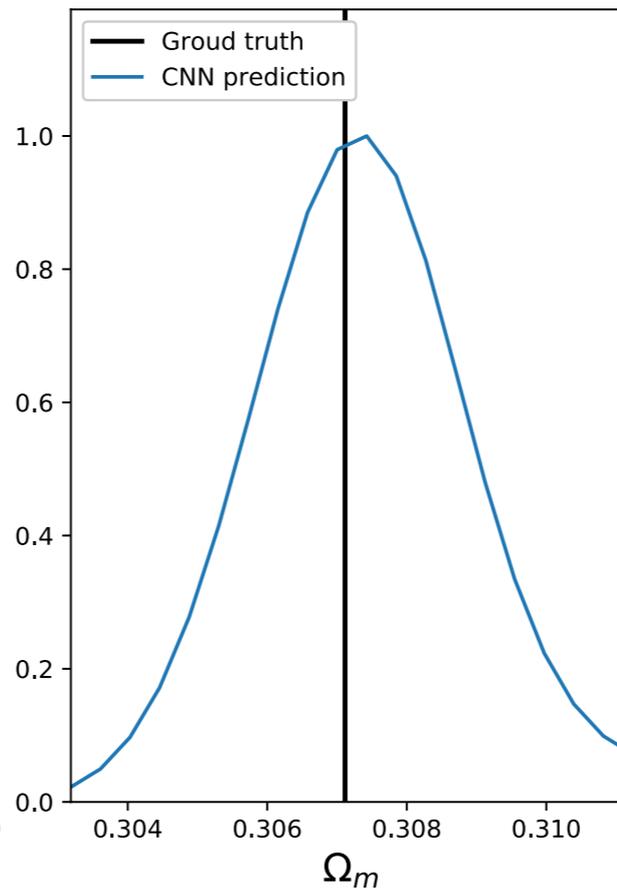
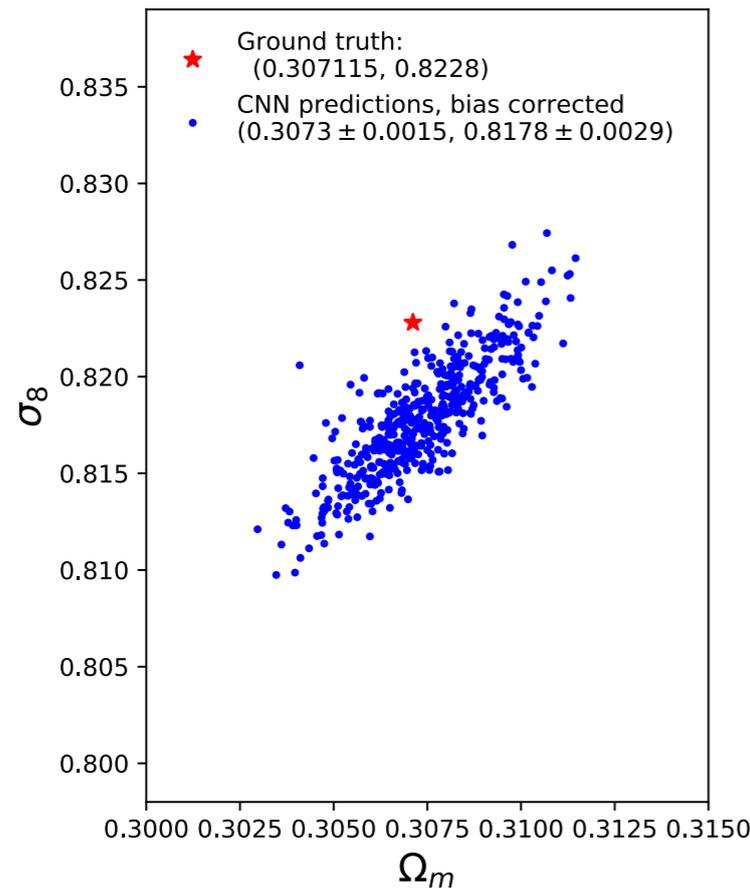
- # of CNN filters
- # of dense neurons
- # of neuron layers
- Optimiser
- Pooling type

Clear advantage in max-pooling over the average pooling

Clear advantage of the SGD optimiser over the default 'Adam' optimiser.

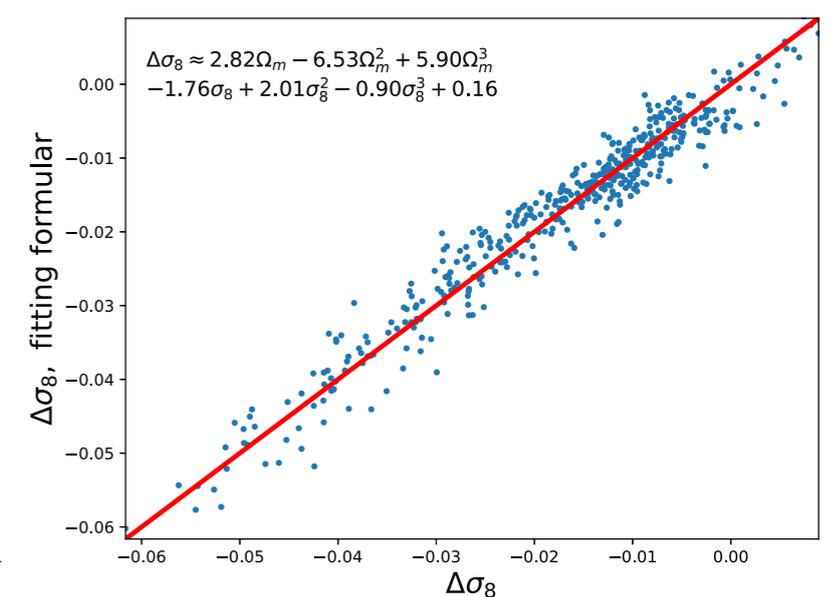
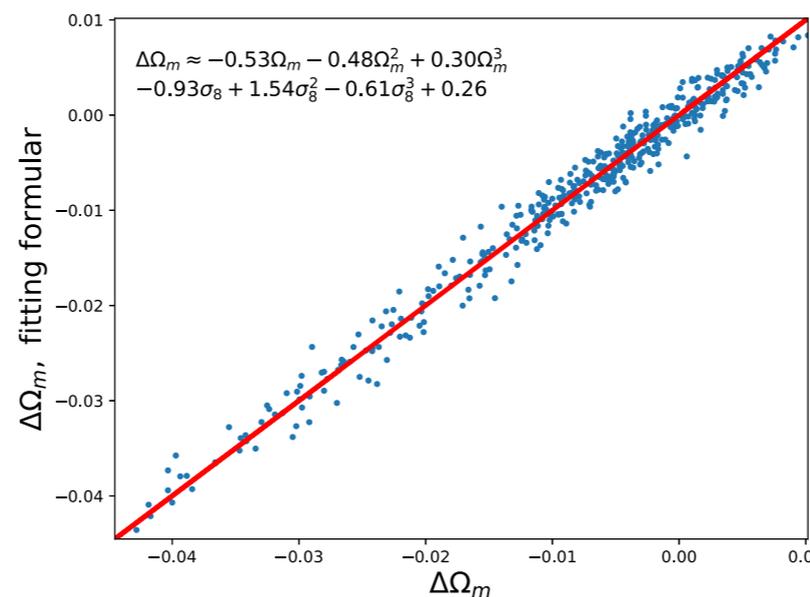


# Deep Learning the Large Scale Structure



We found a significant bias in sigma<sub>8</sub>, this was found in previous works although not really highlighted

It can be easily corrected...



# Deep Learning the Large Scale Structure

---

## CNN adds more information than 2nd order statistics

	Method	Training sample	Relative error of $(\Omega_m, \sigma_8)^a$
Ravanbakhsh et al. (Ravanbakhsh et al. 2017)	CNN	450 simulations $(512 h^{-1}\text{Mpc})^3$ , $512^3$ particles	(0.028, 0.012)
Ravanbakhsh et al. (Ravanbakhsh et al. 2017)	Power spectrum	450 simulations $(512 h^{-1}\text{Mpc})^3$ , $512^3$ particles	(0.072, 0.013)
This work	CNN	465 simulations $(256 h^{-1}\text{Mpc})^3$ , $128^3$ particles	(0.0048, 0.0053)
This work	2pcf, $s \in (0, 130)h^{-1}\text{Mpc}$	465 simulations $(256 h^{-1}\text{Mpc})^3$ , $128^3$ particles	(0.017, 0.012)
This work	2pcf, $s \in (10, 130)h^{-1}\text{Mpc}$	465 simulations $(256 h^{-1}\text{Mpc})^3$ , $128^3$ particles	(0.1, 0.06)

# Deep Learning the Large Scale Structure

---

In collaboration with the Korean Astronomy Machine Learning Group:  
David Parkinson, Sungwook E. Hong, Srivatsan Sridhar, Shi Feng, Sangnam Park, Inku Park, Dongsu Bak, Jacobo Asorey Barreiro, Benjamin L'Hullier, James Jee, Arman Shafieloo, Hanwool Koo, Ryan Keeley +++

- ★ Initiated a project in Korea to further develop this approach
- ★ By considering redshift evolution of the density field we aim to constrain expansion dynamics
- ★ We will consider more realistic tracers such as mock galaxy or weak lensing convergence fields
- ★ We will add systematics such as redshift error, photo-z etc, angular completeness, etc
- ★ How to mitigate nonlinear effects and other small scale physics that are difficult to model - clipping, field transforms, etc

# Information Content from CNN

With Stephen Appleby

But first lets step back and look at Gaussian fields...

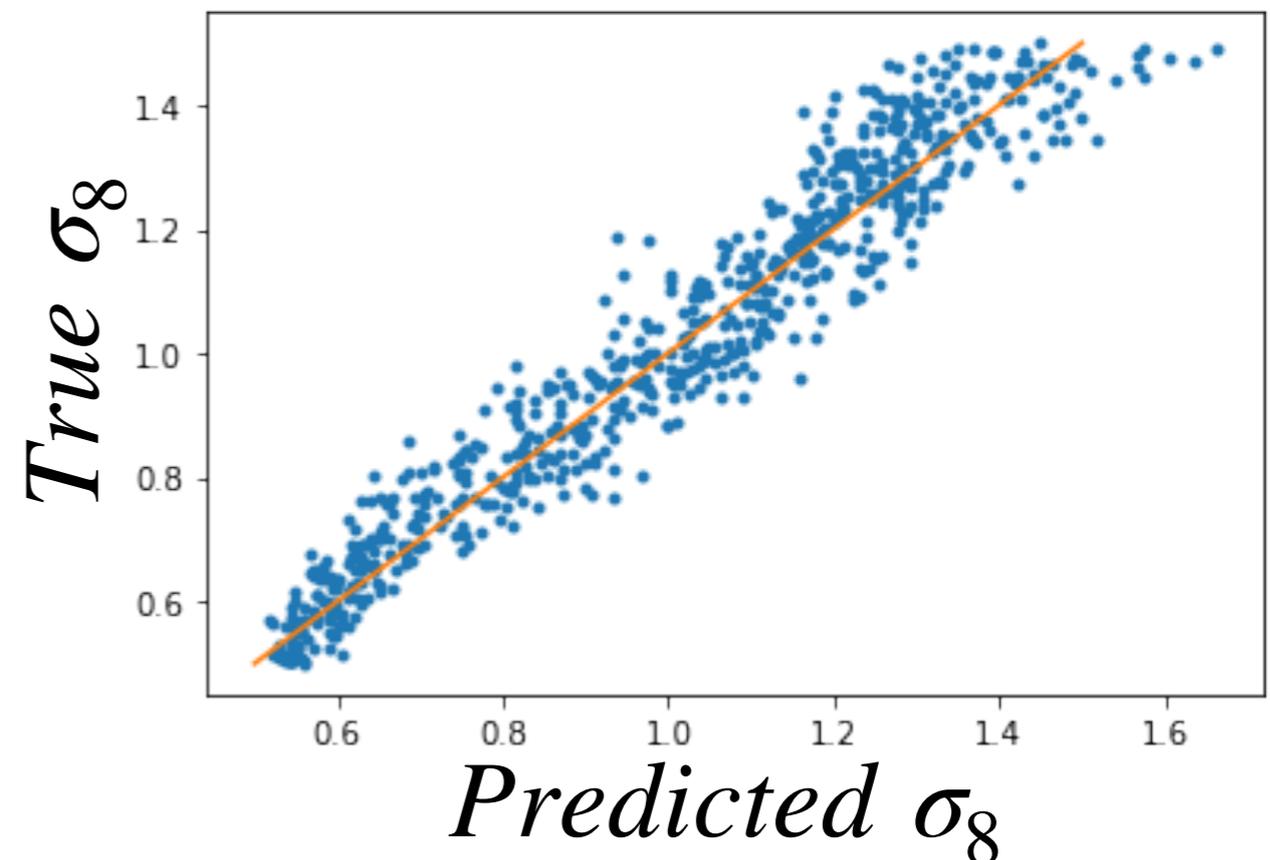
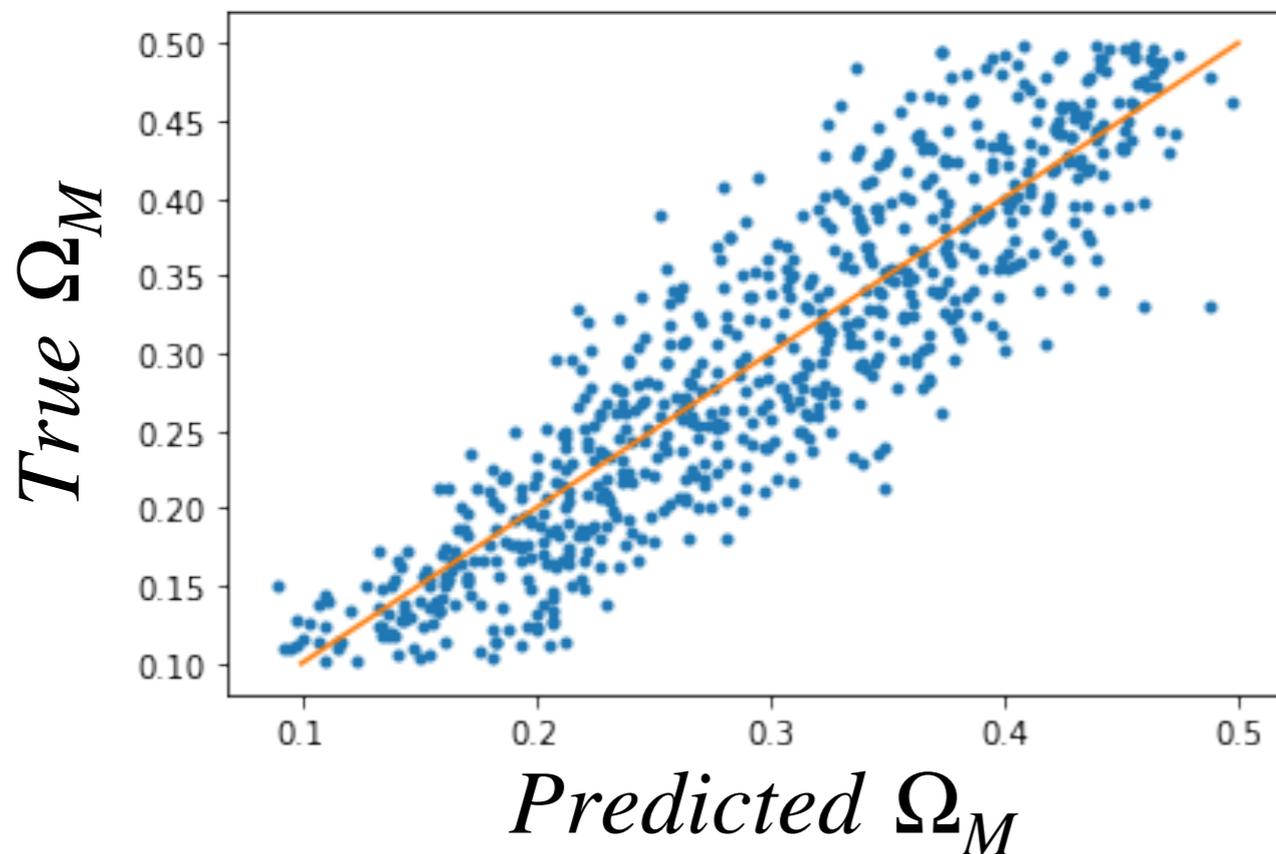
We know that their information is confined to  $\leq 2$ nd order statistics

We can compute the errors on parameters from

- 1) monte carlo realisations
- 2) Fisher matrix

CNN Trained with 6,000 gaussian fields  
with linear cosmological power spectra

Tested below with 600 different fields



# Information Content from CNN

---

With Stephen Appleby

But first lets step back and look at Gaussian fields...

We know that their information is confined to  $\leq 2$ nd order statistics

We can compute the errors on parameters from

- 1) monte carlo realisations
- 2) Fisher matrix
- 3) Via the CNN directly?

We can write a custom loss function,

$$L = \frac{1}{2} \left( \ln (|\Sigma|) + (\theta_p - \theta_t)^T \Sigma^{-1} (\theta_p - \theta_t) \right),$$
$$L = \begin{bmatrix} a & 0 \\ b & c \end{bmatrix} \quad \Sigma^{-1} = LL^T,$$

Where the parameters a,b,c are learned by the network during training.  
The network can learn the covariance matrix directly without an input 'label'

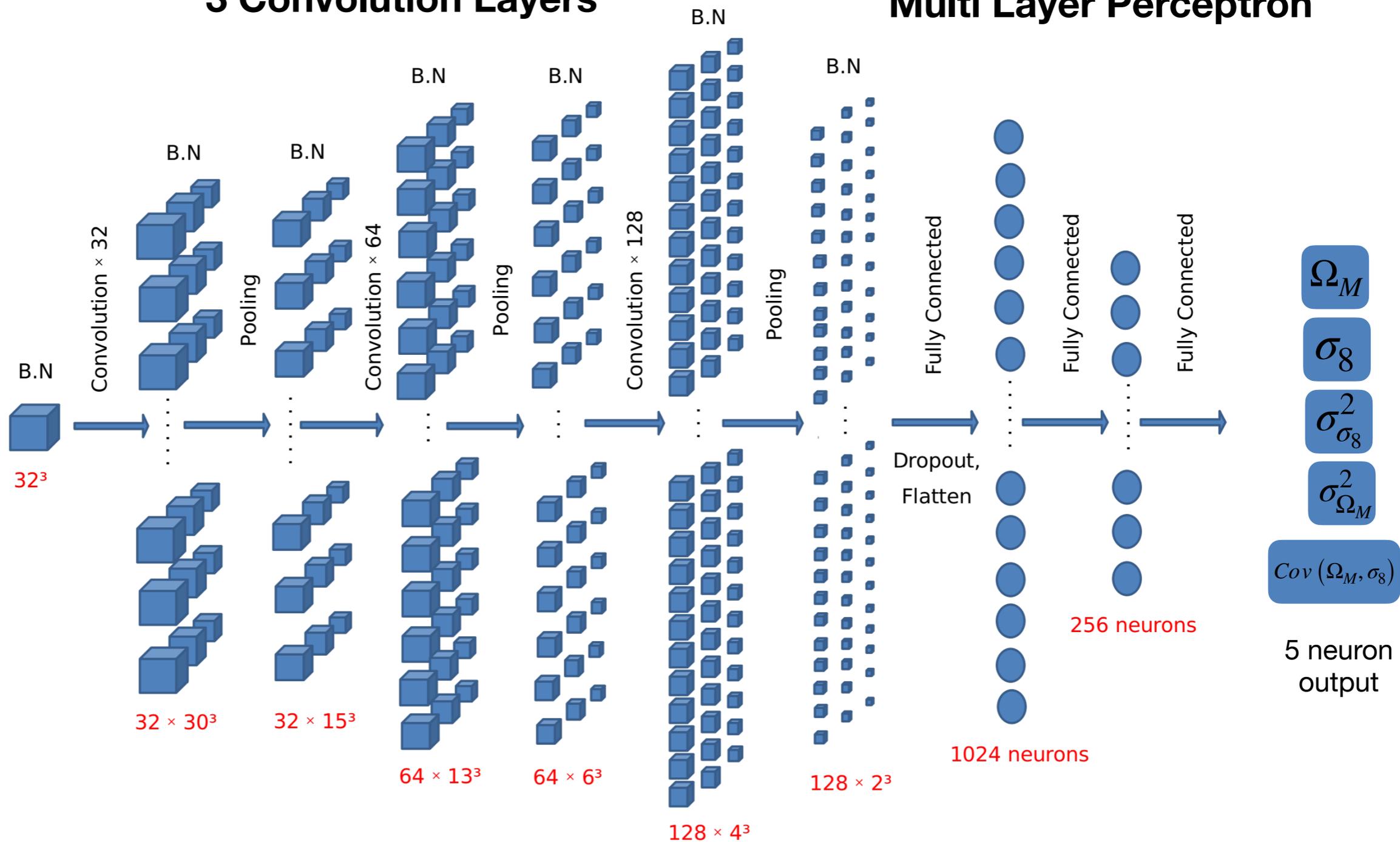
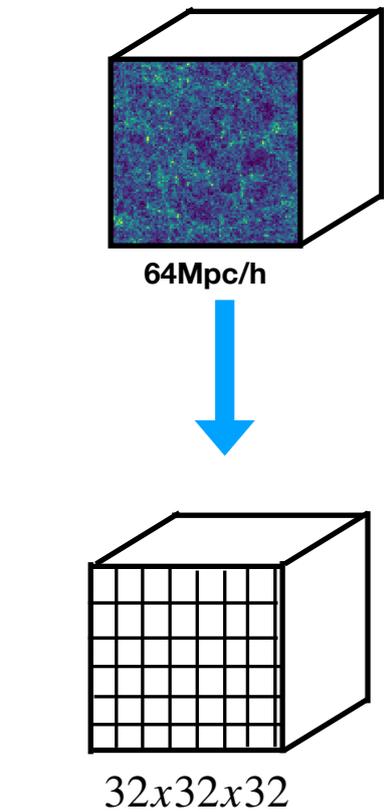
# Information Content from CNN

## Neural Network Architecture

### 3 Convolution Layers

### Multi Layer Perceptron

Cosmic Gaussian field



# Information Content from CNN

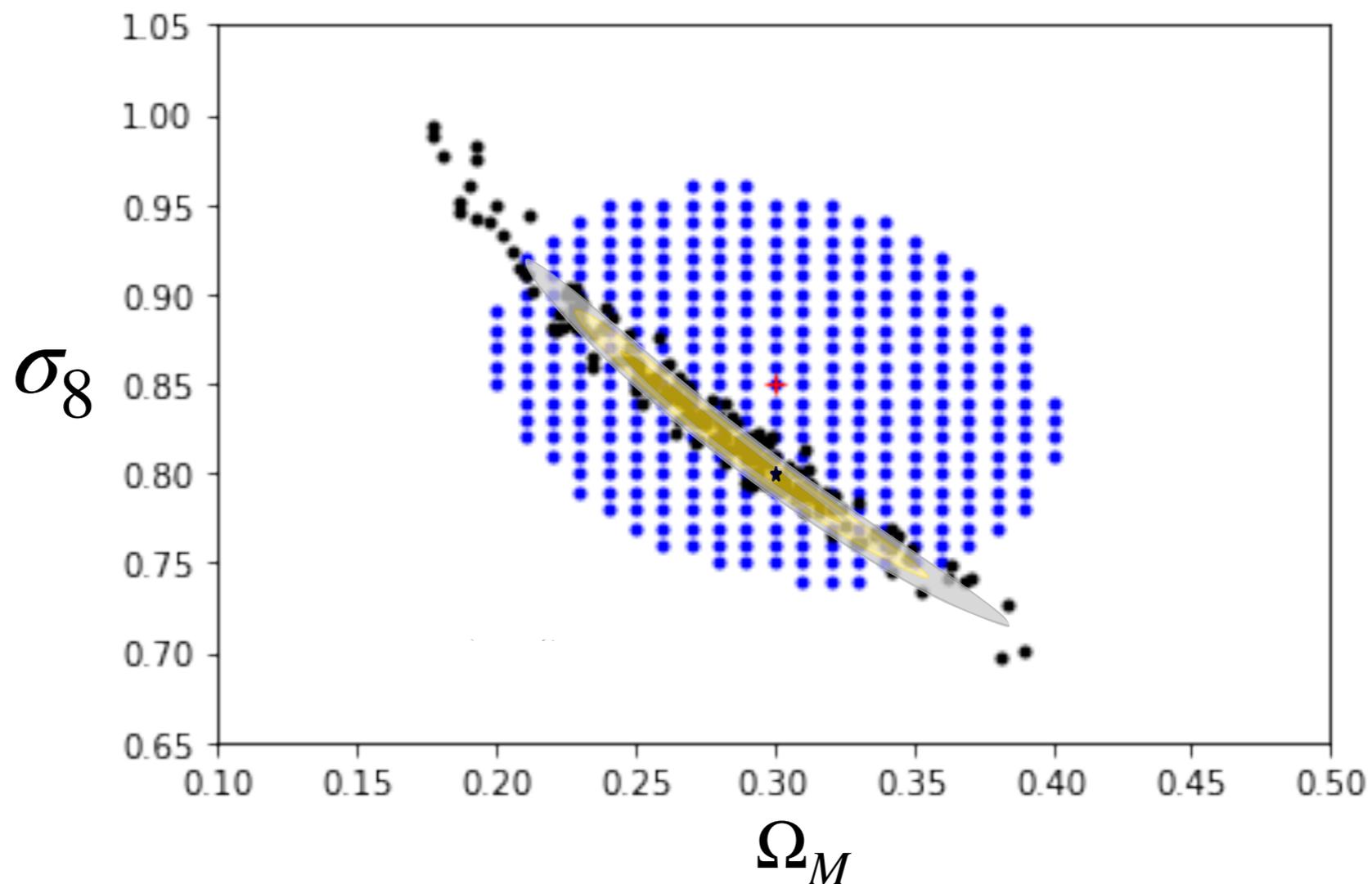
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Stepping back lets looks at Gaussian fields.

We know that their information is confined to  $\leq 2$ nd order statistics

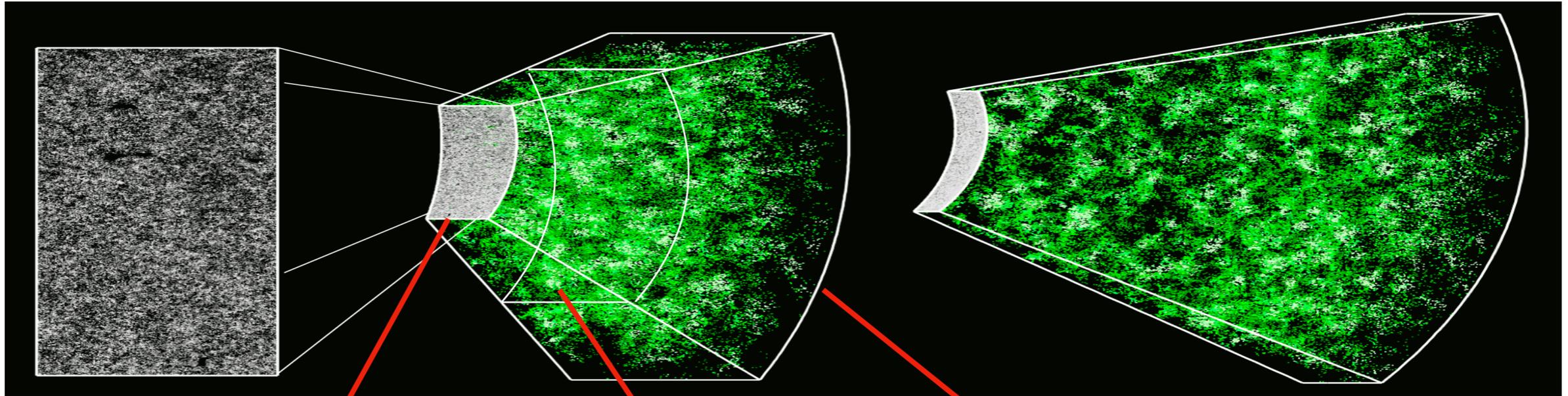
We can compute the errors on parameters from

- 1) monte carlo realisations (black points)
- 2) Fisher matrix (yellow)
- 3) Via the CNN directly (blue)



# Deep Learning the Large Scale Structure

---

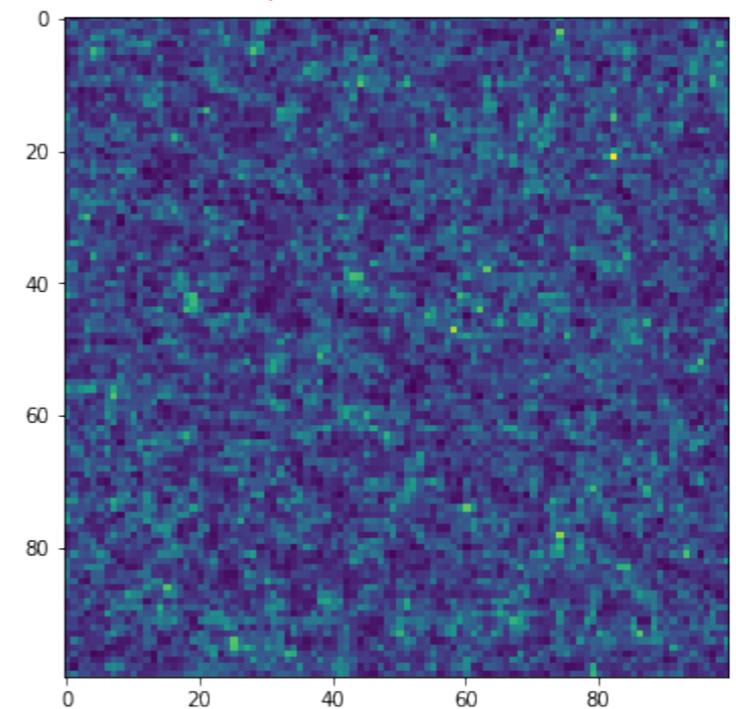
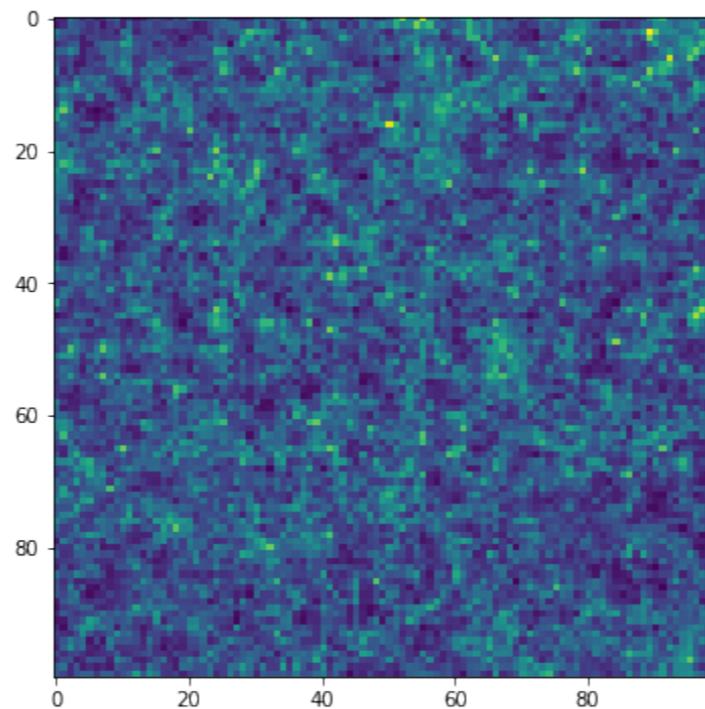
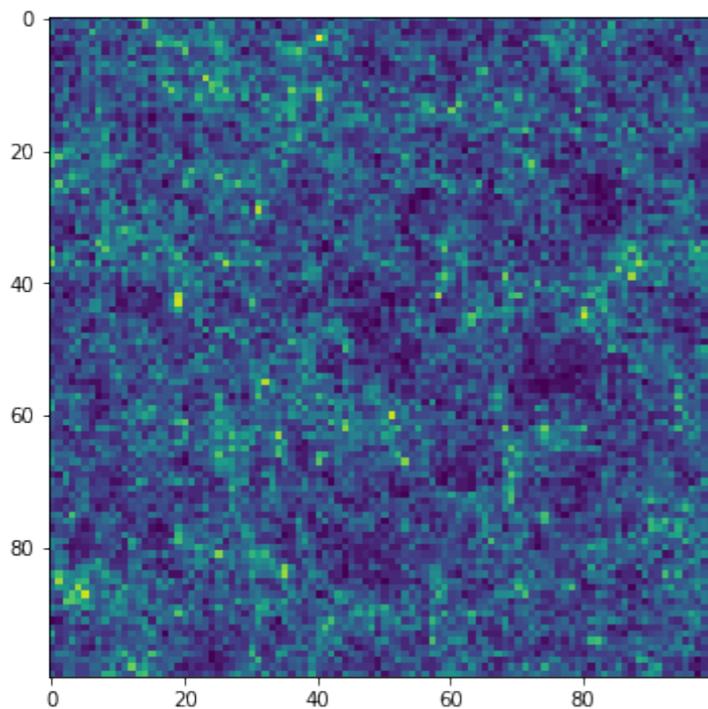


100x100sq deg

**z=0**

**z=1**

**z=2**



# Deep Learning the Large Scale Structure

Fast approx N-body method - Pinocchio Code

2 Gpc/h box,  $1024^3$  particles

FoF halos

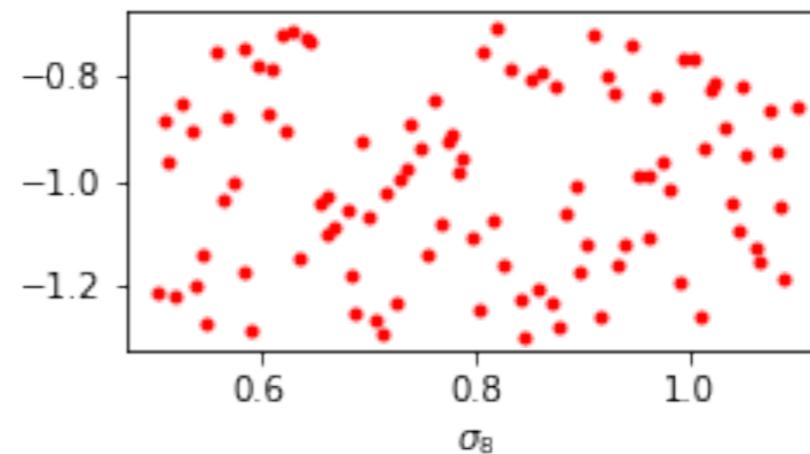
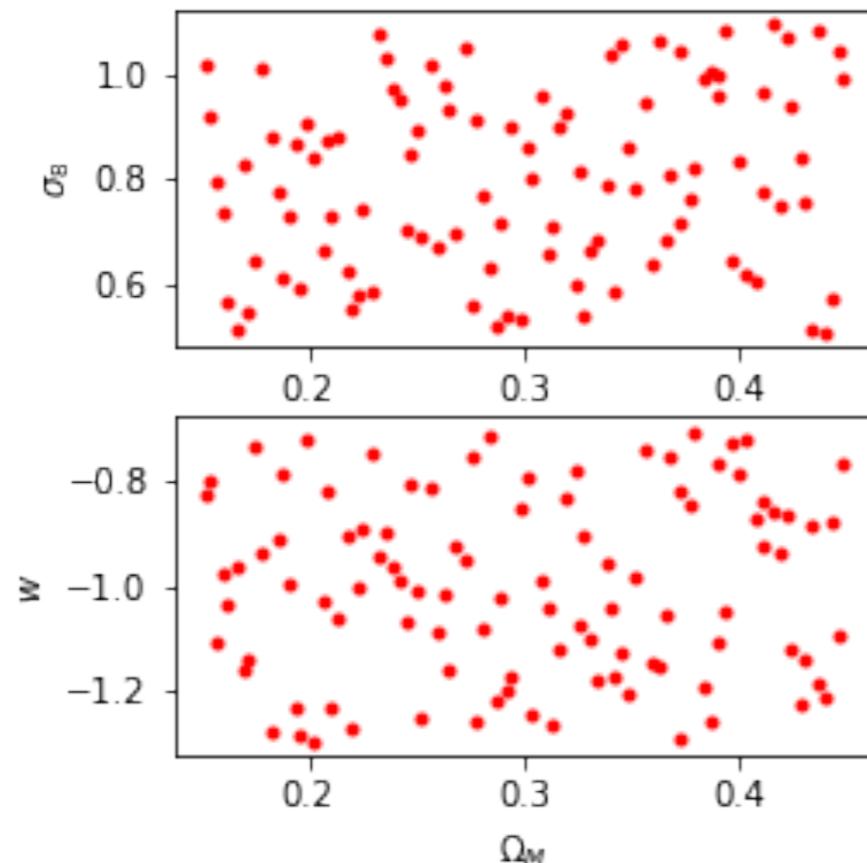
Light-cone output  $0 < z < 2$

6 redshift slices

So far 100 simulations run

Exploring  $\Omega_m$ ,  $s_8$  and  $w$

Parameters sampled from a  
orthogonal Latin Hypercube



Training Data

II

A

X			
	X		
			X
		X	

B

Chess: Rook on each row and file  
without threatening each other

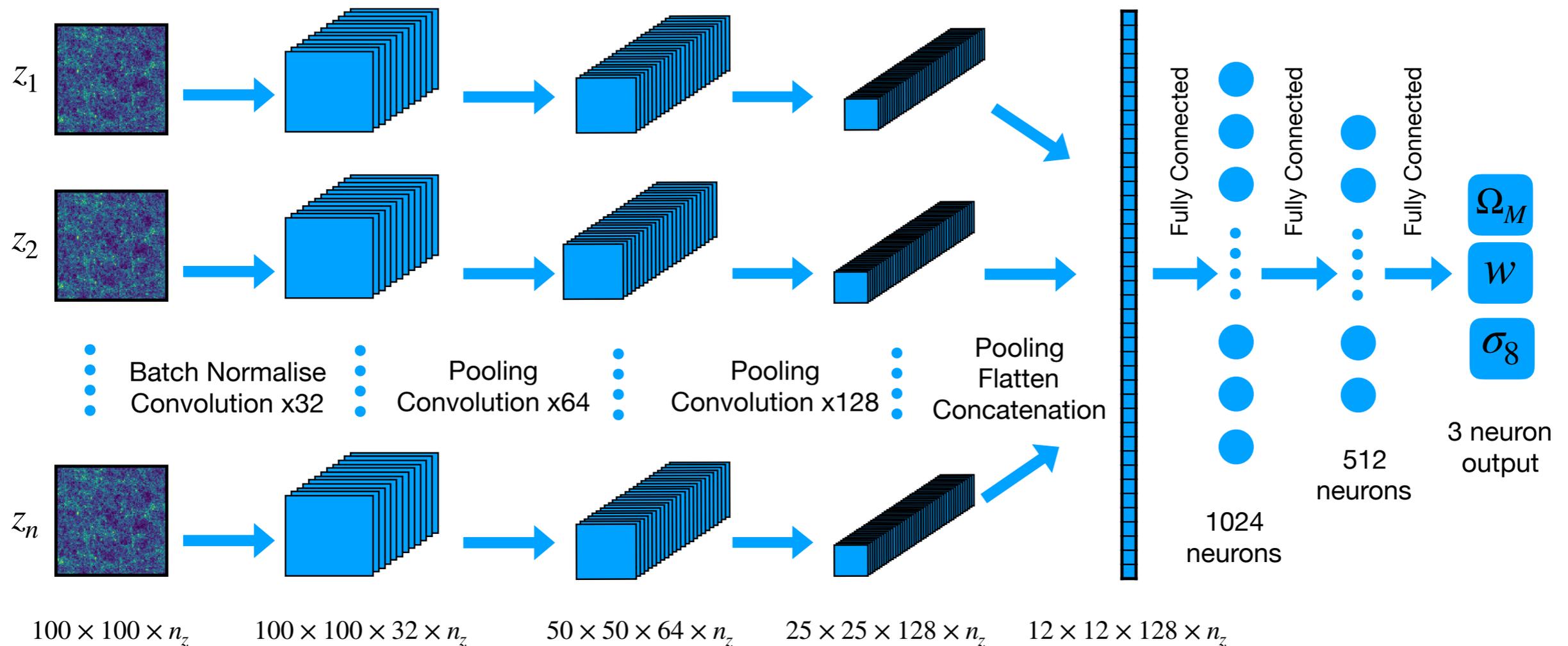
# Deep Learning the Large Scale Structure

## Neural Network Architecture

### Multi Image Input

### Parallel Convolution Layers

### Multi Layer Perceptron

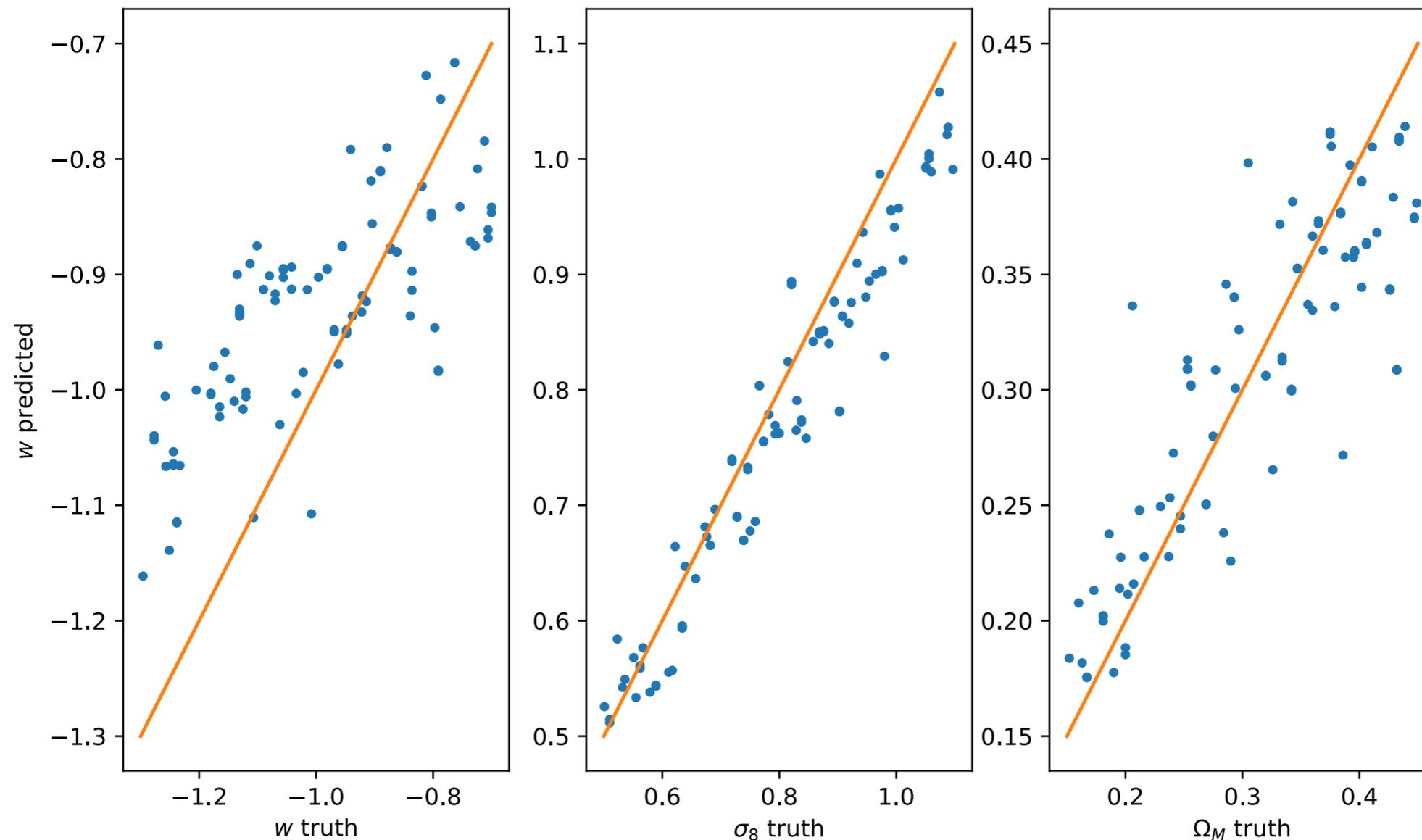


# Deep Learning the Large Scale Structure

## Preliminary Results

### Promising results

- More training data
- Experiment different architecture and hyper parameters
- Test redshift space distortions / photo-z errors / etc



# Deep Learning the Large Scale Structure

---

The Korea Institute of Science and Technology Information (KISTI) Supercomputer Center recently had an open call for proposals specifically aimed at Machine Learning and Big Data.

We were successful and awarded 15 million CPU hours on 'Nurion' (15th fastest in the world)

It is a Cray CS500 system with 570,020 cores



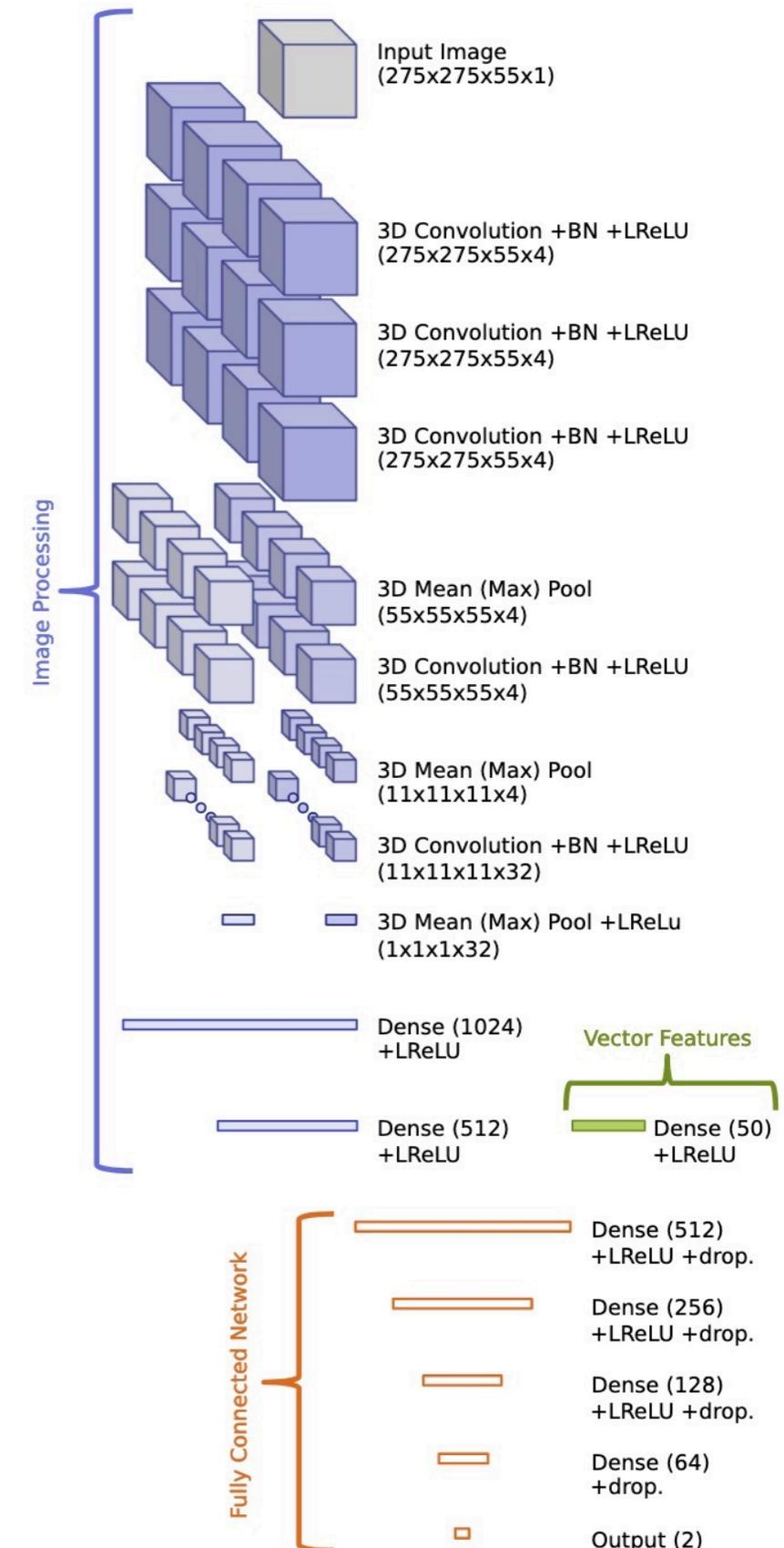
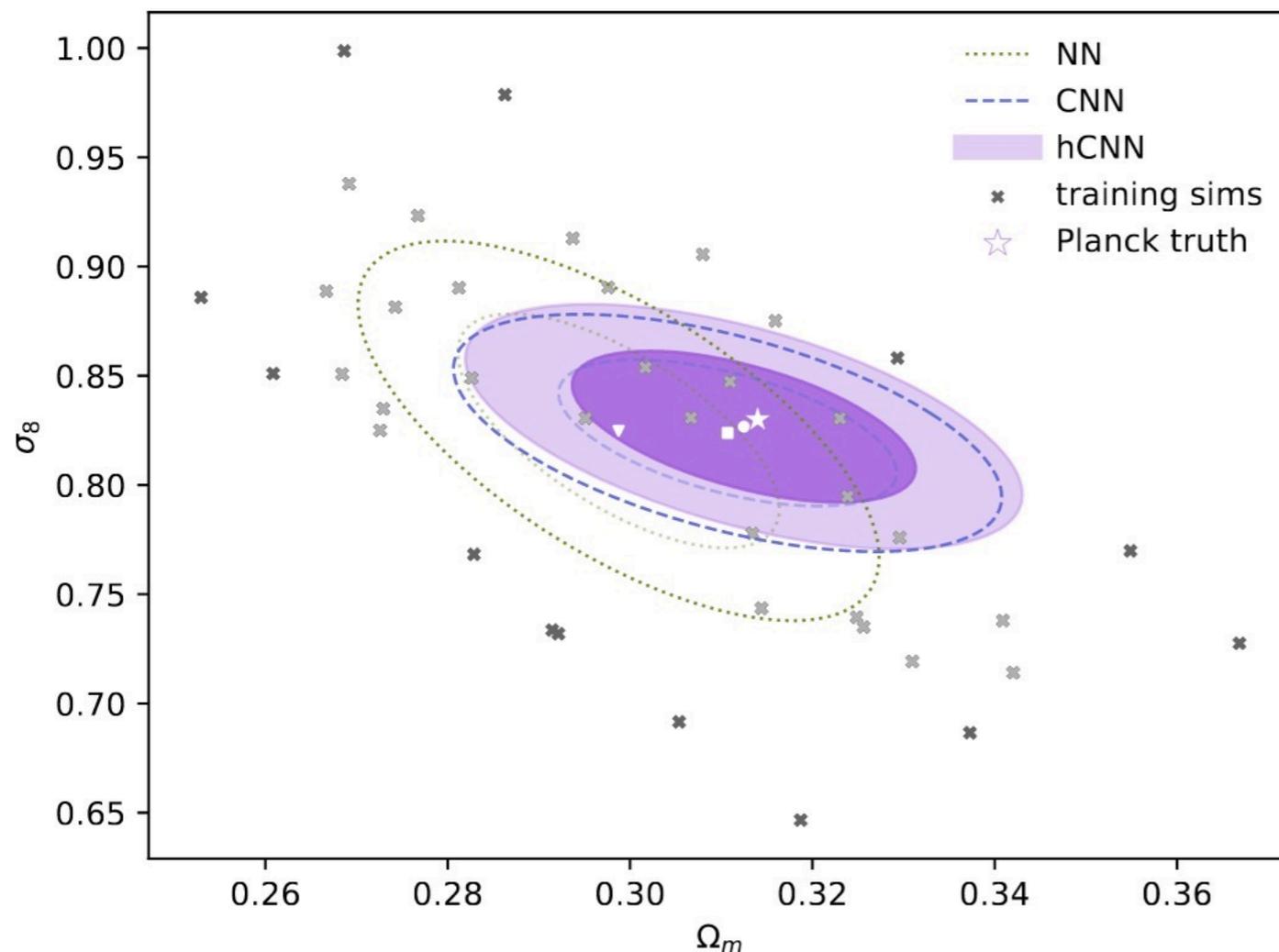
**Proposal:**

- run ~1000 simulations
- Create light-cone cones
- Find halos
- Apply a galaxy assignment model or several models (eg HODs)
- Add observational effects, redshift distortions, photo-z, incompleteness, etc
- Train models and constrain parameters within LCDM
- Apply to observational data, KiDS, SDSS, DLS, early DESI data

# Deep Learning the Large Scale Structure

Ntampaka, Eisenstein, et al. (2019), added mock galaxies to the dark matter halo according to an HOD prescription.

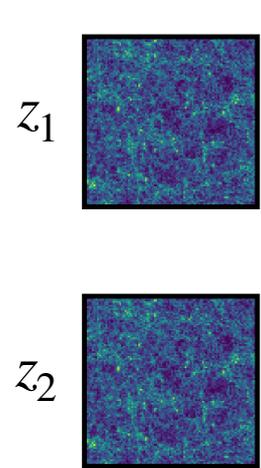
The added 2nd order clustering statistics making a hybrid CNN. But it did not add much information



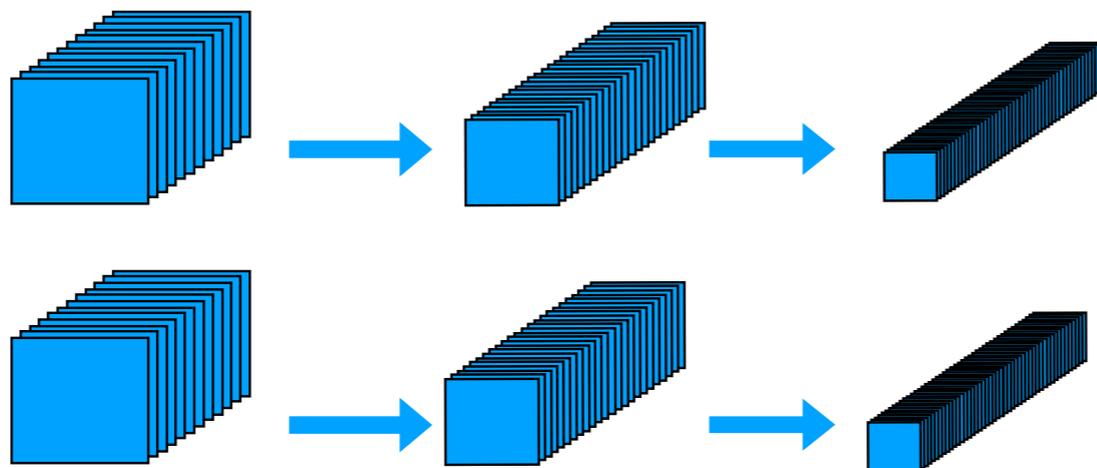
# Deep Learning the Large Scale Structure

## Hybrid Scheme with Higher order statistics

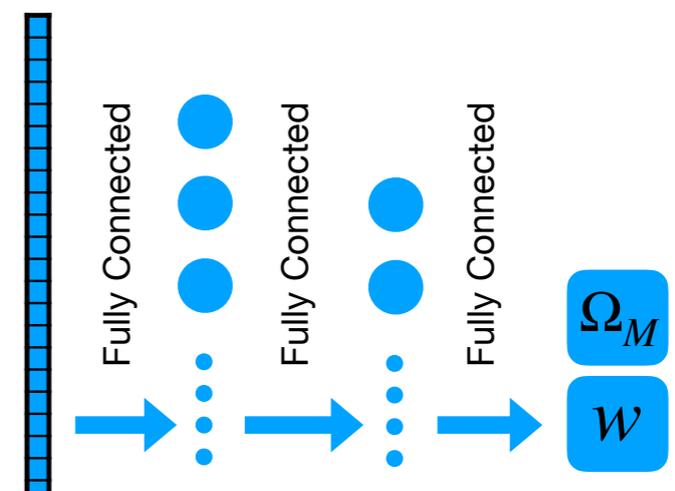
Multi Image Input



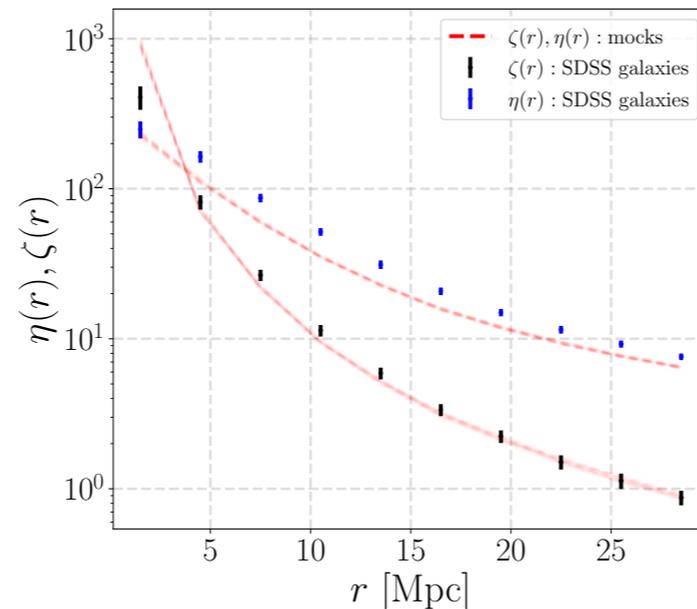
Parallel Convolution Layers



Multi Layer Perceptron



v1 out now!



+



3-pCF

4-pCF

★ C. Sabiu, B. Hoyle, J. Kim, X-D Li

★ <https://arxiv.org/abs/1901.00296> ★ <http://bitbucket.org/csabiu/gramsci>

# Deep Learning the Large Scale Structure

---

- ★ Machine Learning can do as well and potentially better than usual statistical methods for extracting cosmological information from the distribution of galaxies.
- ★ Preliminary results show that CNNs can learn features in the evolving density field to help us constrain parameters including Dark energy and its equation of state,  $w$ .
- ★ Higher Order Statistics beyond the 3rd order can now be computed in a tractable timeframe using graph databases with **GRAMSCI: GRAPh Made Statistics for Cosmological Information** available from: <http://bitbucket.org/csabiu/gramsci>

**Thanks for your attention!**

**Extra**

# Generative Adversarial Networks

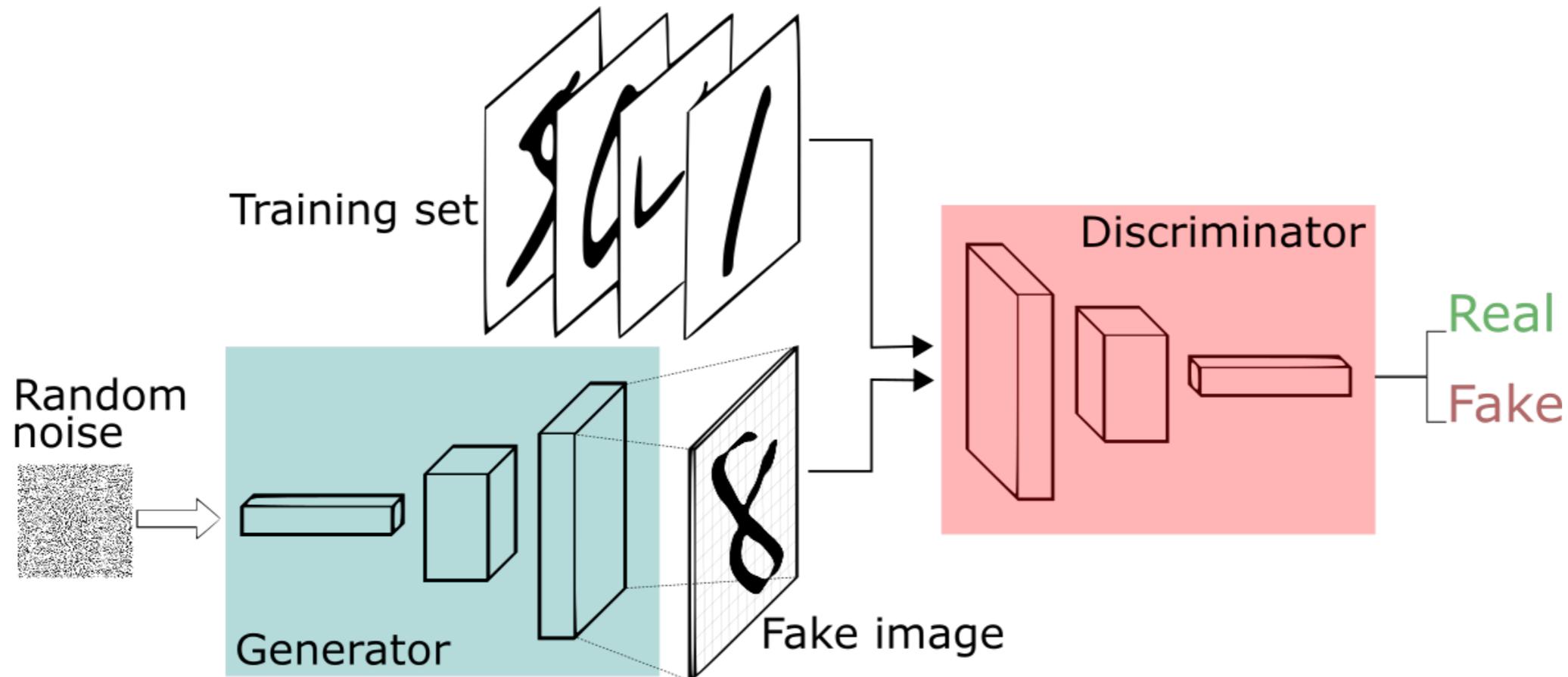


Image credit: [Thalles Silva](#)

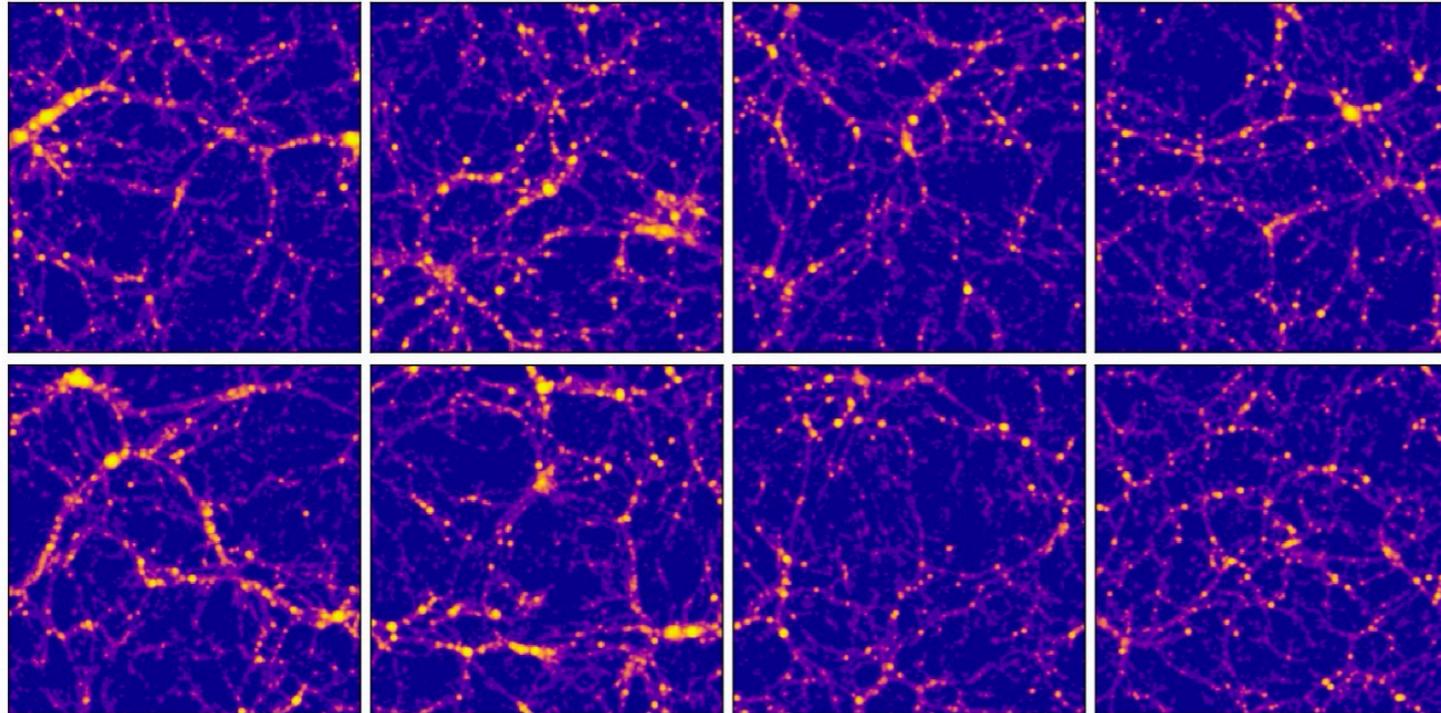
The basic idea behind GANs consists in pairing-up two neural networks: a generator network  $G$  and a discriminator network  $D$ . These networks are trained in an adversarial game setting. The discriminator  $D : \mathbf{x} \mapsto [0; 1]$  tries to probabilistically classify a sample  $\mathbf{x}$  as being real or fake. On the other hand, the generator  $G : \mathbf{z} \mapsto \mathbf{x}$  tries to generate samples that look like they were drawn from the true data distribution  $p_{\text{data}}$ . This generator makes use of a random variable  $\mathbf{z}$  drawn from a given prior  $p_{\text{prior}}(\mathbf{z})$  which is typically a Gaussian distribution. Formally, the two networks  $D$  and  $G$  play the following two-player minimax game:

$$\min_G \max_D [V(D, G)]$$
$$V(D, G) := \mathbb{E}_{\mathbf{x} \sim p_{\text{data}}(\mathbf{x})} [\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim p_{\text{prior}}(\mathbf{z})} [\log(1 - D(G(\mathbf{z})))]$$

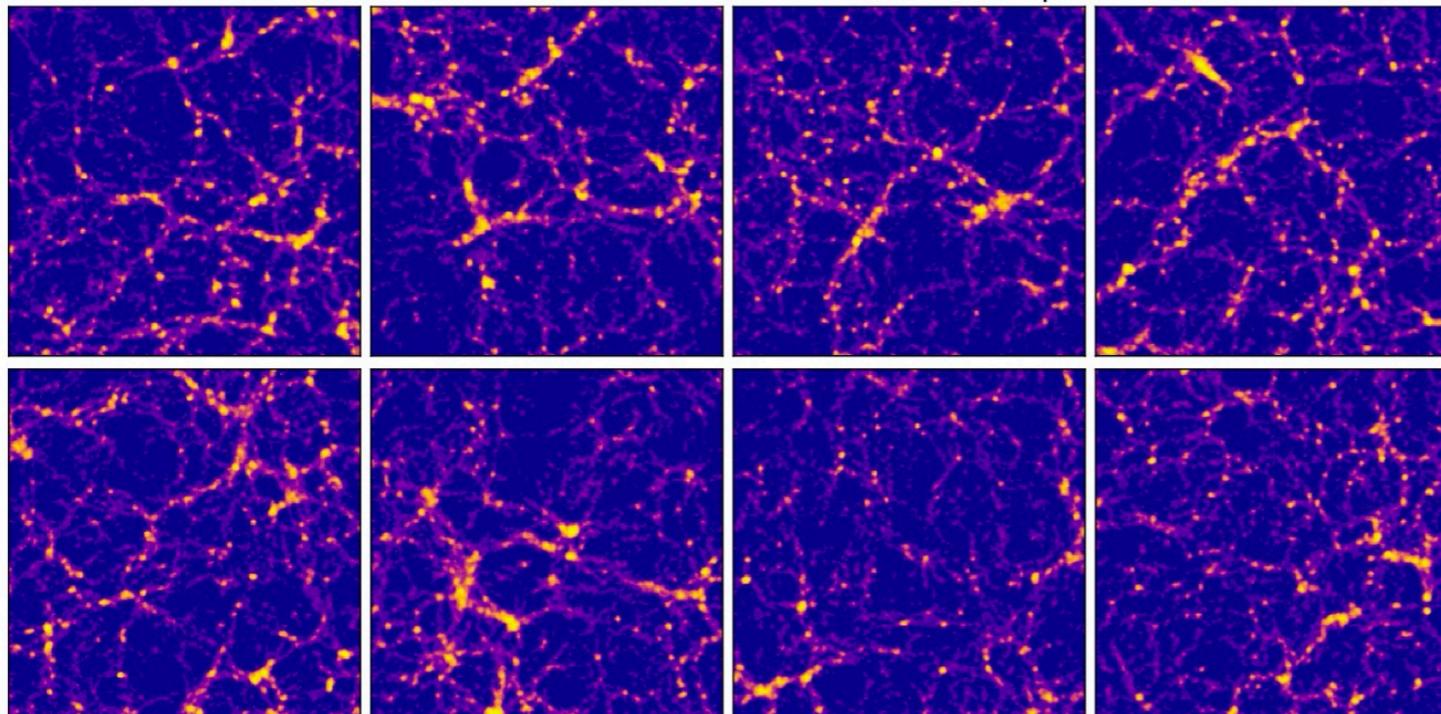
# Generative Adversarial Networks

---

N-body simulation samples

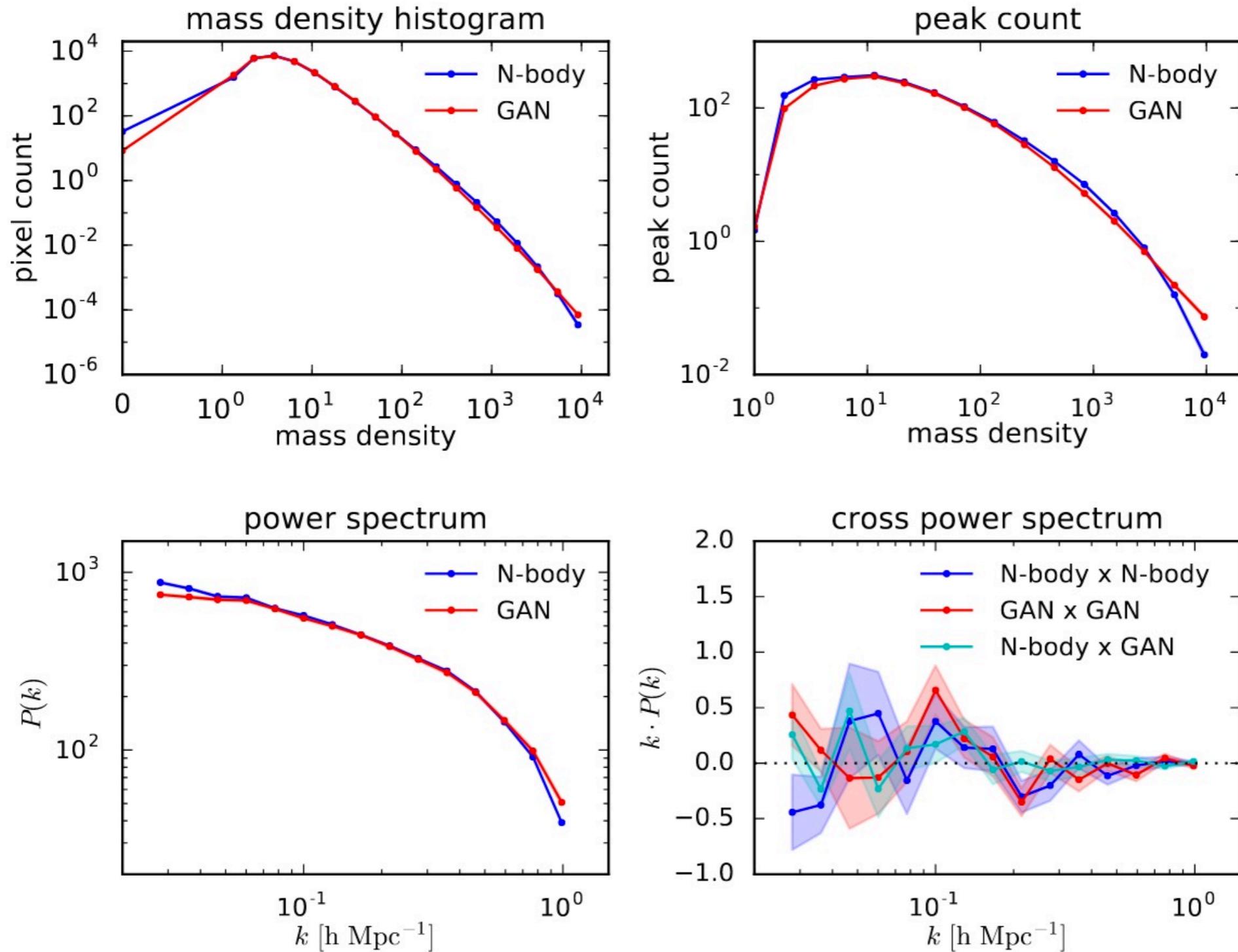


Generative Adversarial Network (GAN) samples



- Optimising a GAN to reproduce N-body density fields of size 100Mpc
- Visually they match very well
- How about the statistics?

# Generative Adversarial Networks



# Galaxy Zoo

<http://zoo1.galaxyzoo.org/>

Members of the public classified galaxies with their eyes (and brains)

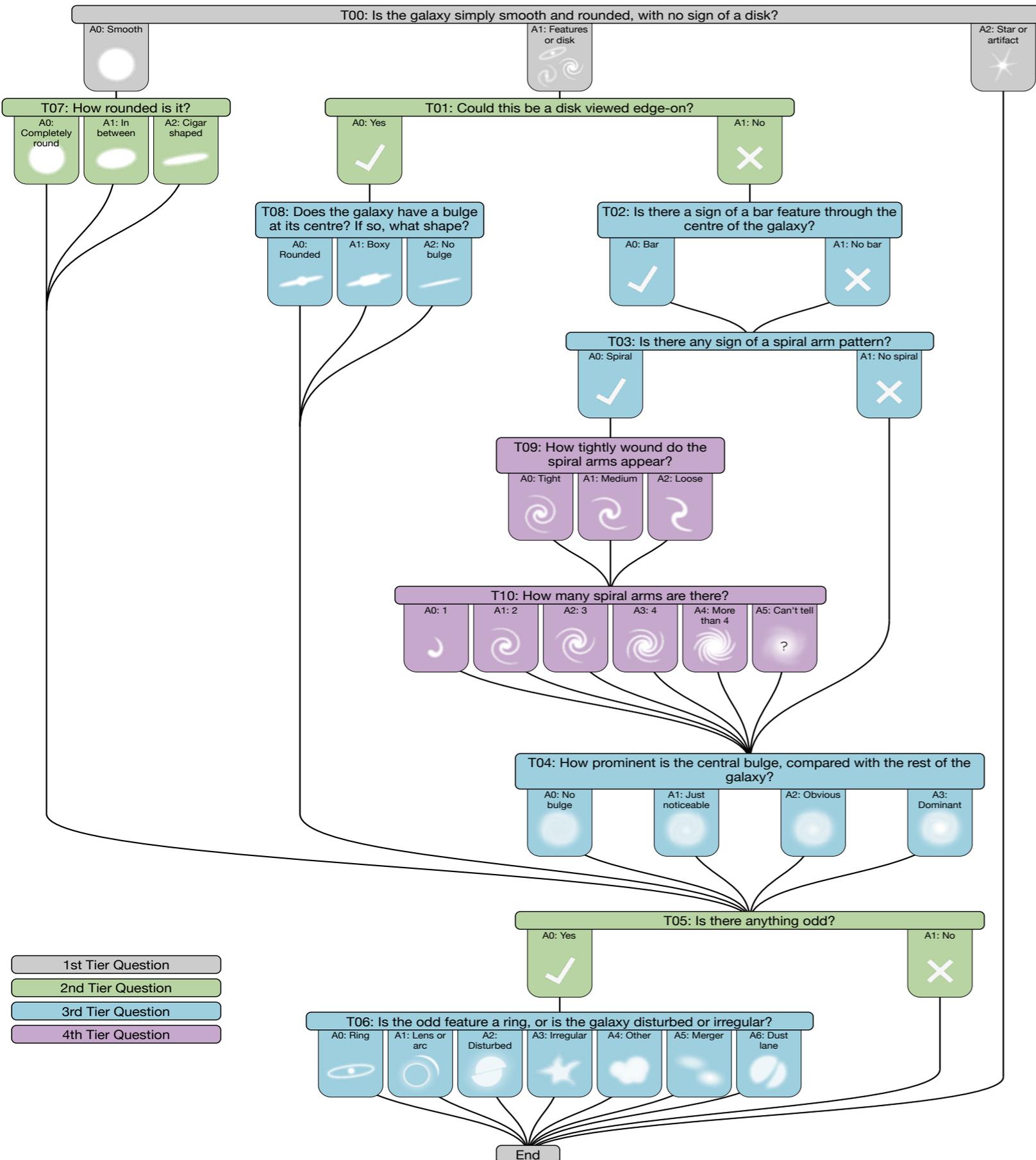
The crowdsourced science project generated a lot of public interest.

1 Million galaxies from SDSS were given multiple classifications

It became possible to do large scale statistics with galaxy morphology!

But the next generation of survey LSST will observe ~37 billion stars and galaxies.

We need a lot more people or use ML!



# Python Example

https://github.com/csabiu/



Pull requests Issues Marketplace Explore



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**kstat**

Fast KD-tree MPI correlation statistics package - Author: Cristiano Sabiu

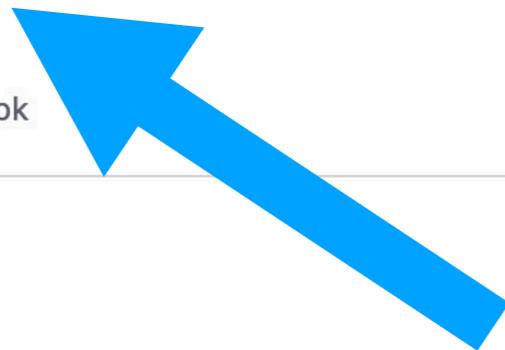
● Fortran

**Gramsci**

GRAph Made Statistics for Cosmological Information

**ML\_tutorial**

● Jupyter Notebook



# Python Example

csabiu / ML\_tutorial

Unwatch 1

★ Star 0

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Code

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# Python Example

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## Import the necessary packages

```
In [1]: # TensorFlow and tf.keras
import tensorflow as tf
from tensorflow import keras

# Helper libraries
import numpy as np
import matplotlib.pyplot as plt
from PIL import Image
import os

print(tf.__version__)
```

1.13.1

Download data sample

# Python Example

[https://colab.research.google.com/github/csabiu/ML\\_tutorial/blob/master/GZ\\_classify.ipynb](https://colab.research.google.com/github/csabiu/ML_tutorial/blob/master/GZ_classify.ipynb)

# Python Example

## shot Import the necessary packages

```
[ ] # TensorFlow and tf.keras
import tensorflow as tf
from tensorflow import keras

# Helper libraries
import numpy as np
import matplotlib.pyplot as plt
from PIL import Image
import os

print(tf.__version__)
```

 1.13.1

## ▾ Download data sample

```
[ ] !wget -q https://github.com/csabiu/ML_tutorial/blob/master/class.tar.gz.parta{a,b,c,d,e,f,g,h,i}?raw=true > tmp
!cat class.tar.gz.parta*true > class.tar.gz
!gunzip class.tar.gz
!tar -xvf class.tar > tmp
!rm class.tar*
!rm tmp
!ls
```

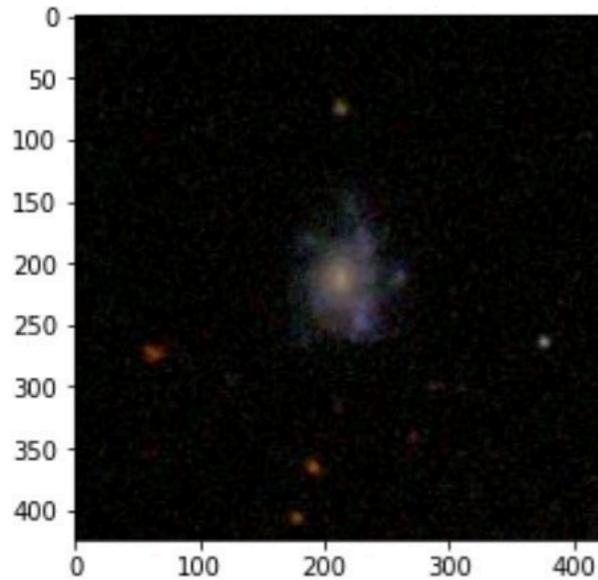
 class sample\_data

# Python Example

## ▼ Lets look at an image

```
shot  
jpgfile = Image.open("class/100134.jpg")  
plt.imshow(jpgfile)  
print(np.shape(jpgfile))
```

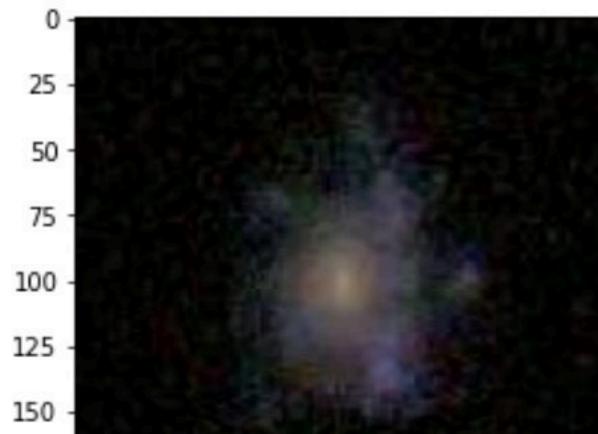
(424, 424, 3)



## ▼ Lets crop it

```
[ ] plt.imshow(jpgfile.crop((112,112,312,312)))
```

<matplotlib.image.AxesImage at 0x7f3662676208>

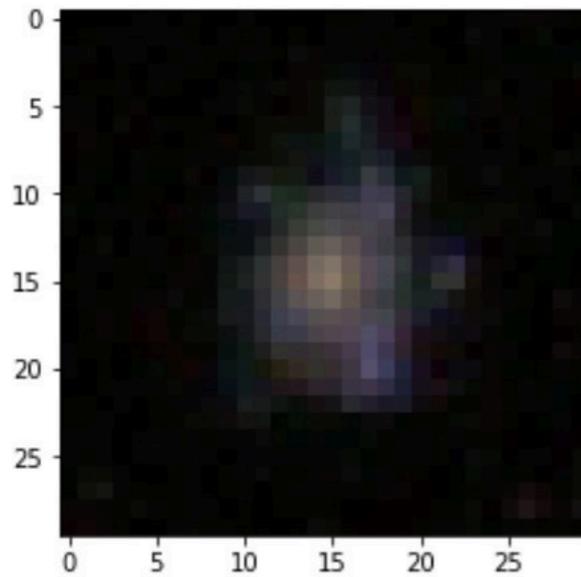


# Python Example

## And lower the resolution

```
shot plt.imshow(jpgfile.crop((112,112,312,312)).resize((30,30),Image.ANTIALIAS))
```

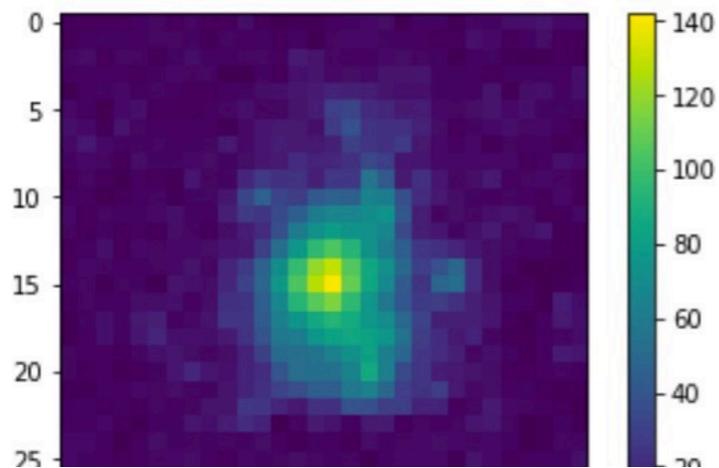
<matplotlib.image.AxesImage at 0x7f3660e4eeb8>



## Split into RGB colors

```
[ ] r,g,b=jpgfile.split()  
plt.imshow(r.crop((112,112,312,312)).resize((30,30),Image.ANTIALIAS))  
plt.colorbar()
```

<matplotlib.colorbar.Colorbar at 0x7f3660d58dd8>



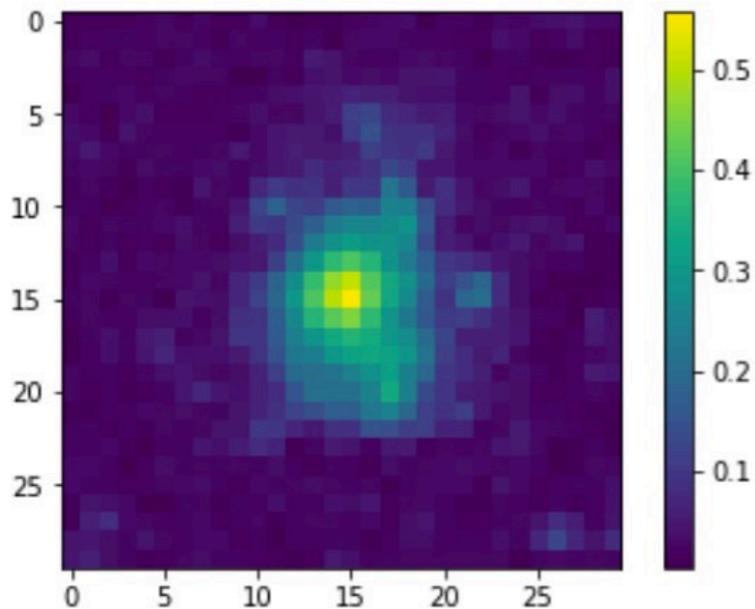
# Python Example

## ▾ Normalise the pixel values to (0,1)

shot

```
im=np.zeros((30,30))
im[:,:]=r.crop((112,112,312,312)).resize((30,30),Image.ANTIALIAS)
im=im/255.
plt.imshow(im)
plt.colorbar()
```

 <matplotlib.colorbar.Colorbar at 0x7fe7907426a0>



## ▾ Load the labels (truth) data

(Image ID, galaxy type) - 0=smooth, 1=featured

```
[ ] data=np.loadtxt("class/truth.txt",dtype='i')
print(np.shape(data))
labels=data[:,1]

print(data[1:10,:]) # print first 10 entries
```

 (16885, 2)  
[[100134 1]  
 [100322 1]

# Python Example

## ↳ Lets transform all the images and save into an array

shot

```
[ ] images=np.zeros((16885,30,30,3))
nn=0

for i in (data[:,0]):
    filename=str(int(i))+".jpg"
    jpgfile = Image.open("./class/"+filename)
    images[nn,:,:,:]=jpgfile.crop((112,112,312,312)).resize((30,30),Image.ANTIALIAS)
    nn=nn+1

images=images/255.
print(np.shape(images))
```

 (16885, 30, 30, 3)

## ↳ Split images and labels into training and test data

```
[ ] images=images.mean(axis=3) # average colour -> greyscale
train_data=images[:13000,:,:]
test_data=images[13000,:,:]

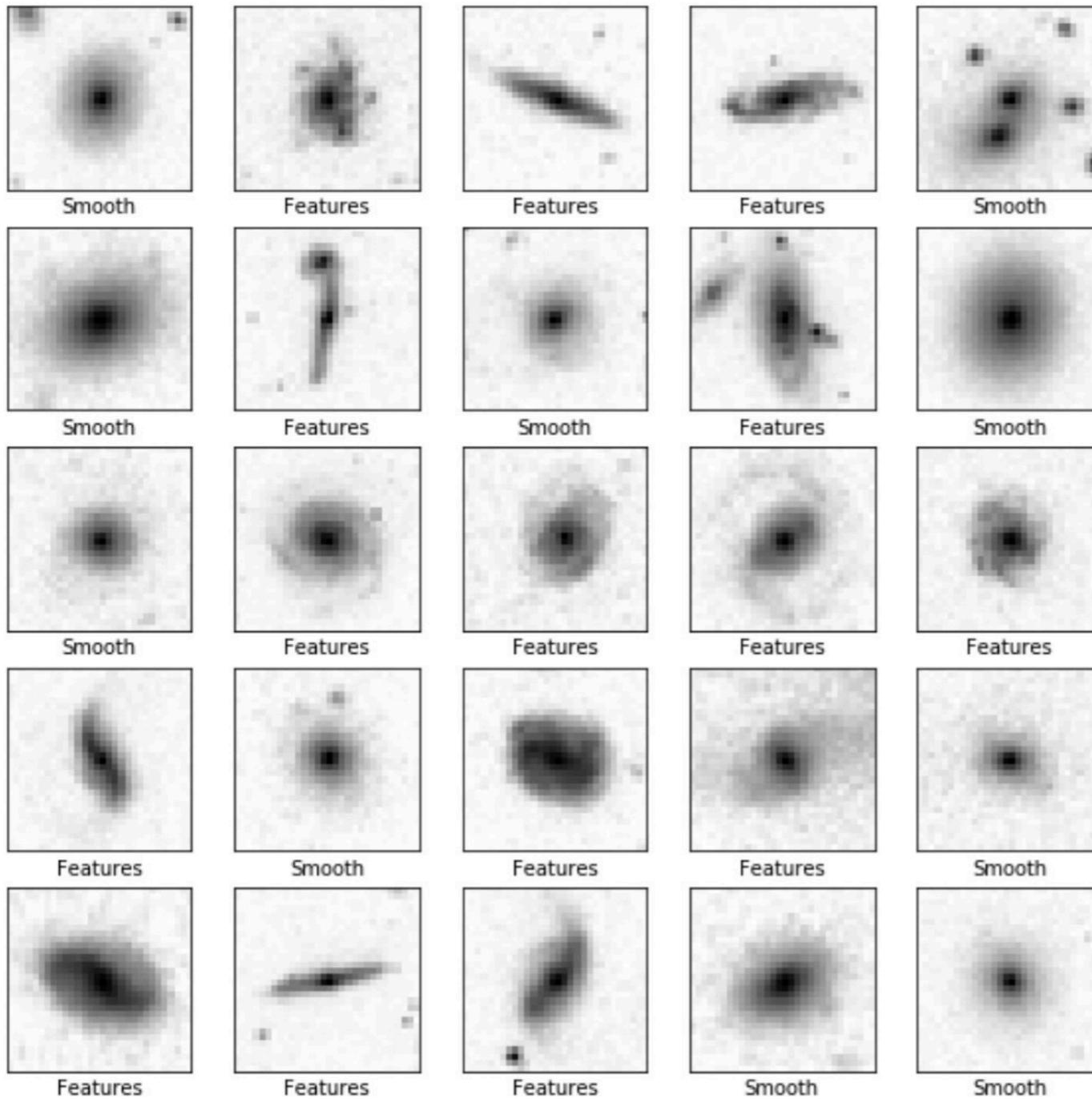
train_label=labels[:13000]
test_label=labels[13000:]

print(np.shape(train_data))
print(np.shape(train_label))
print(np.shape(test_data))
print(np.shape(test_label))
```

 (13000, 30, 30)  
(13000,)  
(3885, 30, 30)  
(3885,)

# Python Example

```
[ ] class_names = ['Smooth', 'Features']  
plt.figure(figsize=(10,10))  
for i in range(25):  
    plt.subplot(5,5,i+1)  
    plt.xticks([])  
    plt.yticks([])  
    plt.grid(False)  
    plt.imshow(train_data[i], cmap=plt.cm.binary)  
    plt.xlabel(class_names[int(train_label[i])])  
plt.show()
```



# Python Example

## ▾ Define a simple neural network

shot

```
[ ] from keras.utils.vis_utils import plot_model
keras.backend.clear_session()
model = keras.Sequential([
    keras.layers.Flatten(input_shape=(30, 30)),
    keras.layers.Dense(64, activation=tf.nn.relu),
    keras.layers.Dense(2, activation=tf.nn.softmax)])
model.summary()

model.compile(optimizer='adam',
              loss='sparse_categorical_crossentropy',
              metrics=['accuracy'])
```

 WARNING:tensorflow:From /usr/local/lib/python3.6/dist-packages/tensorflow/Instructions for updating:  
Colocations handled automatically by placer.  
Using TensorFlow backend.

Layer (type)	Output Shape	Param #
flatten (Flatten)	(None, 900)	0
dense (Dense)	(None, 64)	57664
dense_1 (Dense)	(None, 2)	130

=====  
Total params: 57,794  
Trainable params: 57,794  
Non-trainable params: 0  
=====

# Python Example

```
[ ] model.fit(train_data[:,:,:], train_label, epochs=7)
```

Epoch 1/7

13000/13000 [=====] - 1s 96us/sample - loss: 0.5173 - acc: 0.7727

Epoch 2/7

13000/13000 [=====] - 1s 72us/sample - loss: 0.4068 - acc: 0.8407

Epoch 3/7

13000/13000 [=====] - 1s 73us/sample - loss: 0.3689 - acc: 0.8573

Epoch 4/7

13000/13000 [=====] - 1s 72us/sample - loss: 0.3510 - acc: 0.8630

Epoch 5/7

13000/13000 [=====] - 1s 74us/sample - loss: 0.3323 - acc: 0.8722

Epoch 6/7

13000/13000 [=====] - 1s 74us/sample - loss: 0.3243 - acc: 0.8740

Epoch 7/7

13000/13000 [=====] - 1s 73us/sample - loss: 0.3088 - acc: 0.8816

<tensorflow.python.keras.callbacks.History at 0x7fe790509080>

```
[ ] test_loss, test_acc = model.evaluate(test_data[:,:,:], test_label)
print('Test accuracy:', test_acc)
```

3885/3885 [=====] - 0s 46us/sample - loss: 0.3299 - acc: 0.8798

Test accuracy: 0.87979406

# Python Example

## ▾ Make predictions on test data from the trained model

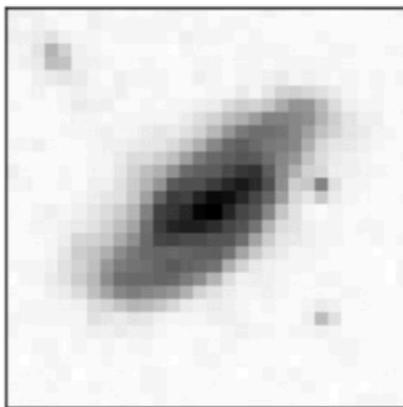
shot

```
[ ] predictions = (model.predict(test_data[:, :, :]))  
  
print("First 10 galaxies")  
print("Predicted:", np.argmax(predictions[1:11], axis=1))  
print("Truth:      ", np.int_(test_label[1:11]))
```

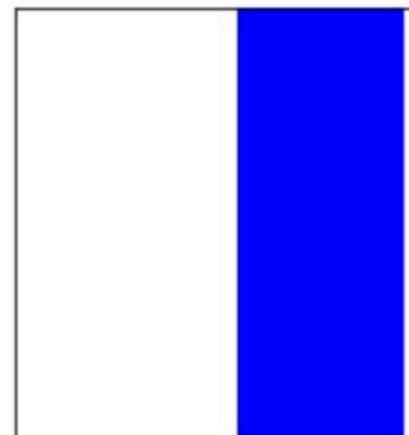
👤 First 10 galaxies  
Predicted: [1 1 1 1 1 1 1 0 0 1]  
Truth: [1 1 0 1 0 1 1 0 1 1]

## ▾ Lets visualise these classifications

```
[ ] i = 4  
plt.figure(figsize=(6,3))  
plt.subplot(1,2,1)  
plot_image(i, predictions, np.int_(test_label), test_data)  
f=plt.subplot(1,2,2)  
plot_value_array(i, predictions, np.int_(test_label))  
f.axes.set_xticklabels(["smooth", "features"])  
plt.show()
```

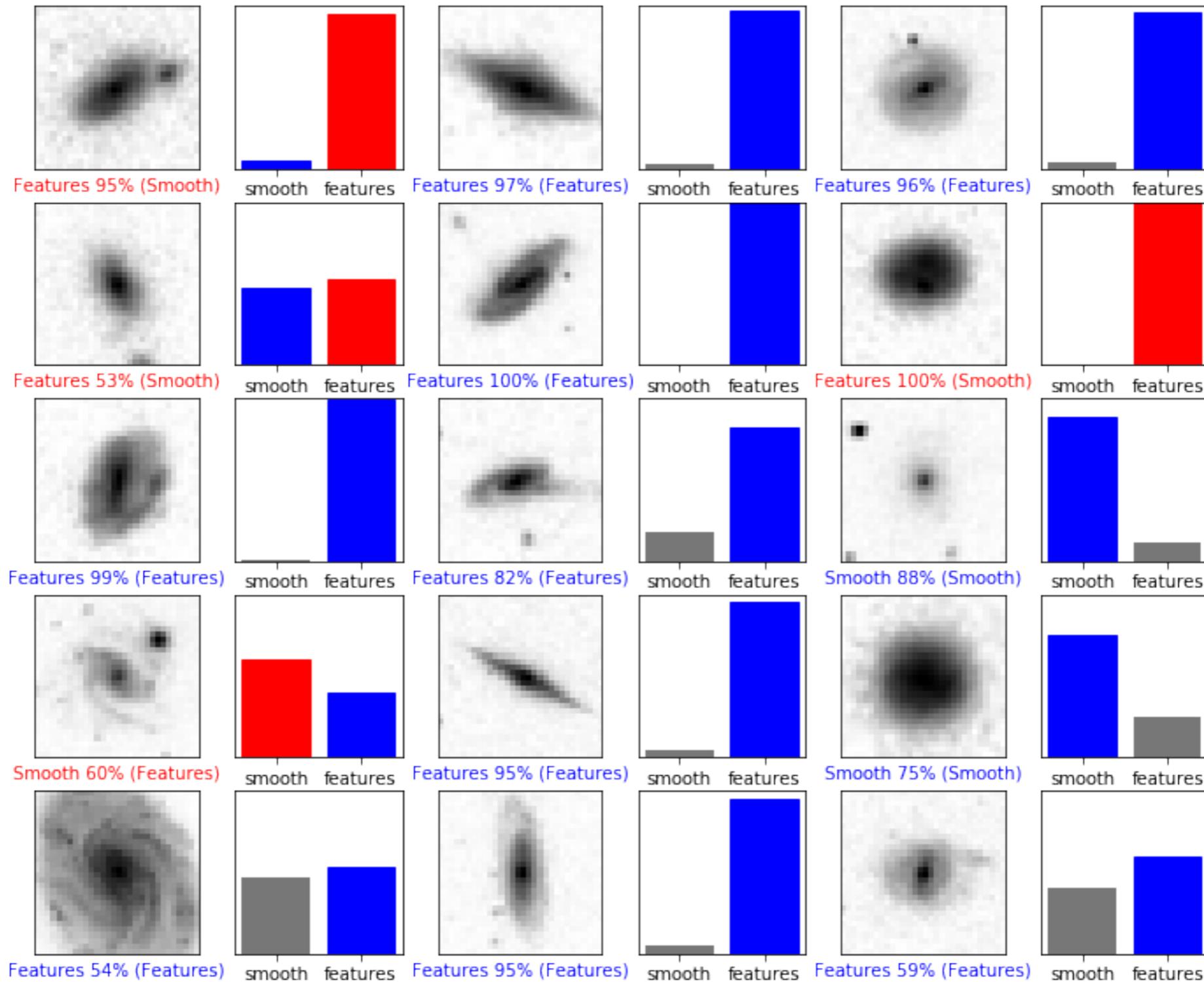


Features 100% (Features)



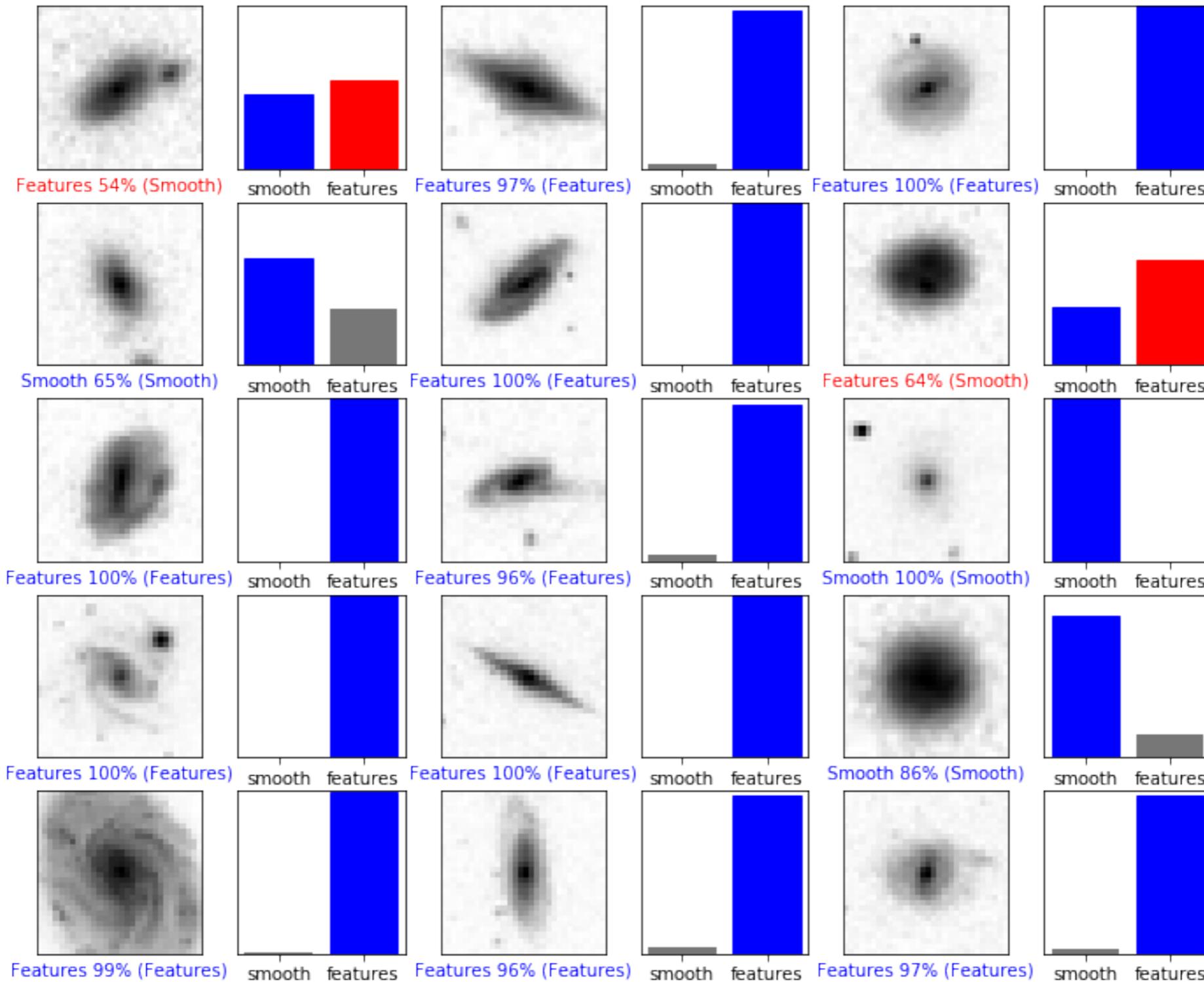
smooth features

# Python Example



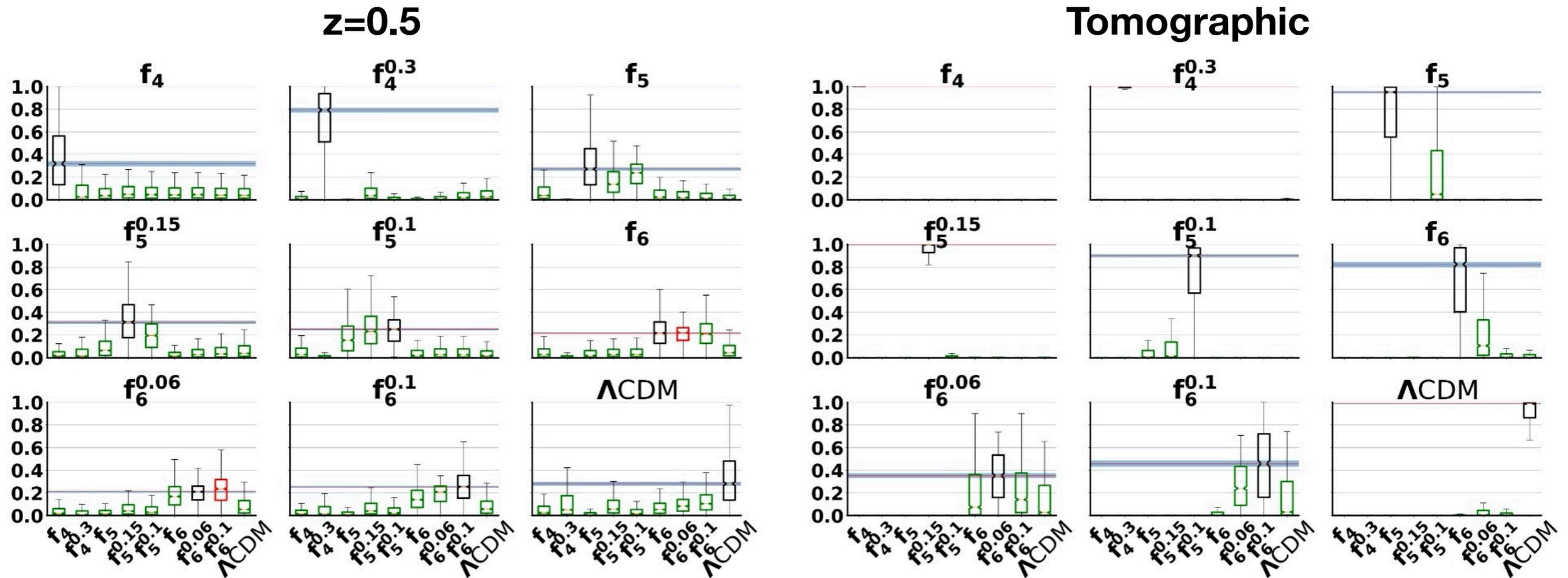
# Python Example

Now using a convolutional neural network!



# Deep Learning the Large Scale Structure

CNN applied to Convergence maps in fR gravity

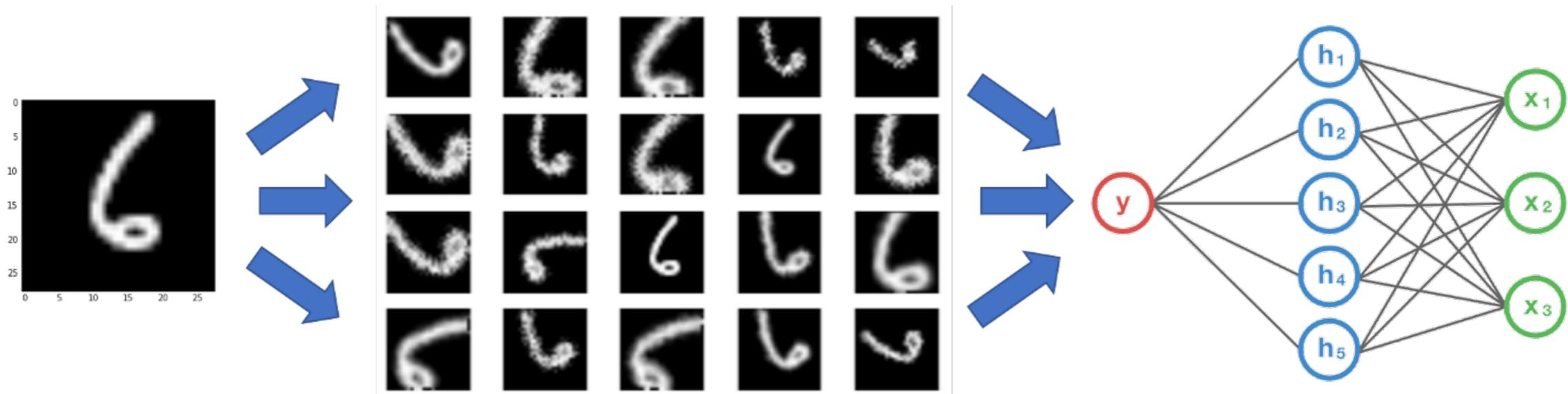


Julian Merten, et al 2019 (arXiv:1810.11027)

# Convolutional Neural Networks

## Data Augmentation

A convolutional neural network that can robustly classify objects even if its placed in different orientations is said to have the property called **invariance**. More specifically, a CNN can be invariant to translation, viewpoint, size or illumination (Or a combination of the above).

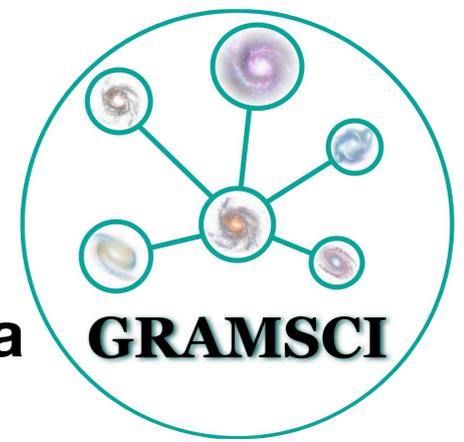


### Popular augmentations:

- left/right flip
- up/down flip
- Random rotation
- Zoom scale
- Crop
- X,Y translation (shift)

# Conclusions

---



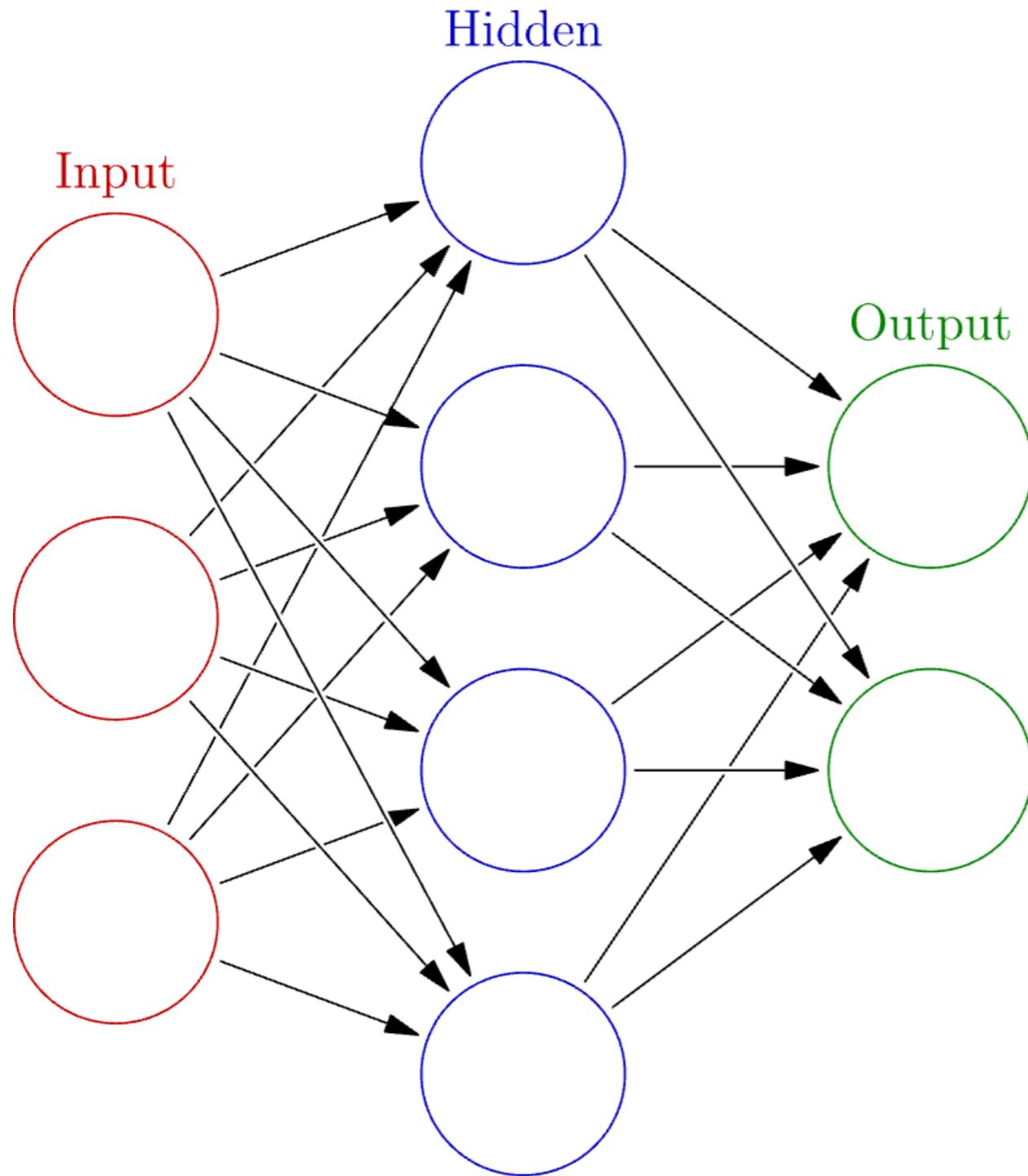
- ★ We introduce a new clustering algorithm, publicly available under a GNU public release licence
- ★ **GRA**ph **M**ade **S**tatistics for **C**osmological **I**nformation: **GRAMSCI** available from: <http://bitbucket.org/csabiu/gramsci>
- ★ GRAMSCI performs much better than purely tree based approaches
- ★ We show the performance by measuring all possible 3pCF unto and beyond the BAO scale with current SDSS BOSS data
- ★ We make the first measurements of the 4-point function of SDSS galaxies
- ★ We show the flexibility of adopting a Big Data Analytic approach. As an example the luminosity-number density cross correlation has the potential to unlock new information in the galaxy data that depends on baryonic physics and compensated isocurvature originating in the very early Universe.

**v1 out now!**

**Thank You 감사합니다**

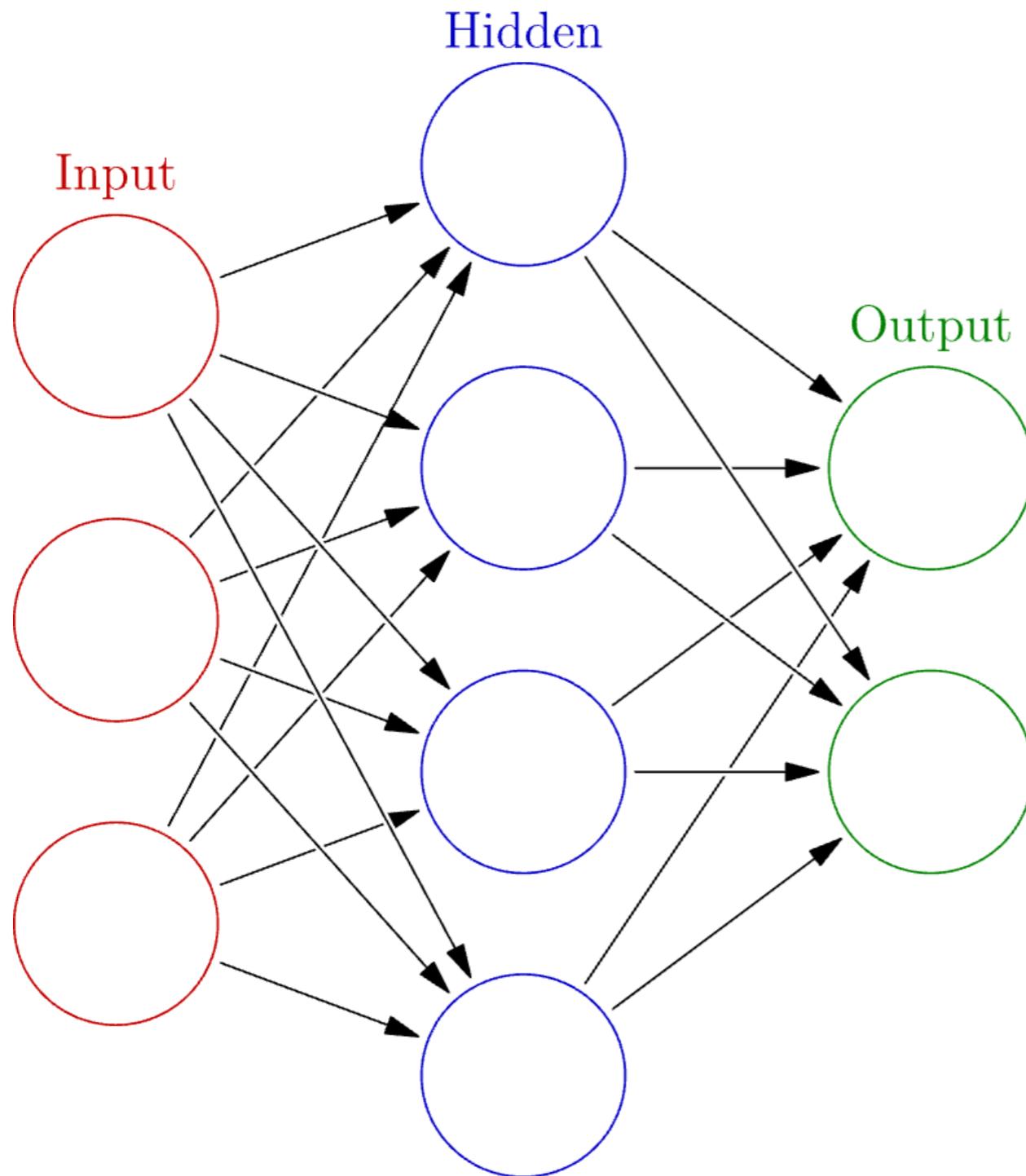
# Artificial Neural Networks

---



# Artificial Neural Networks

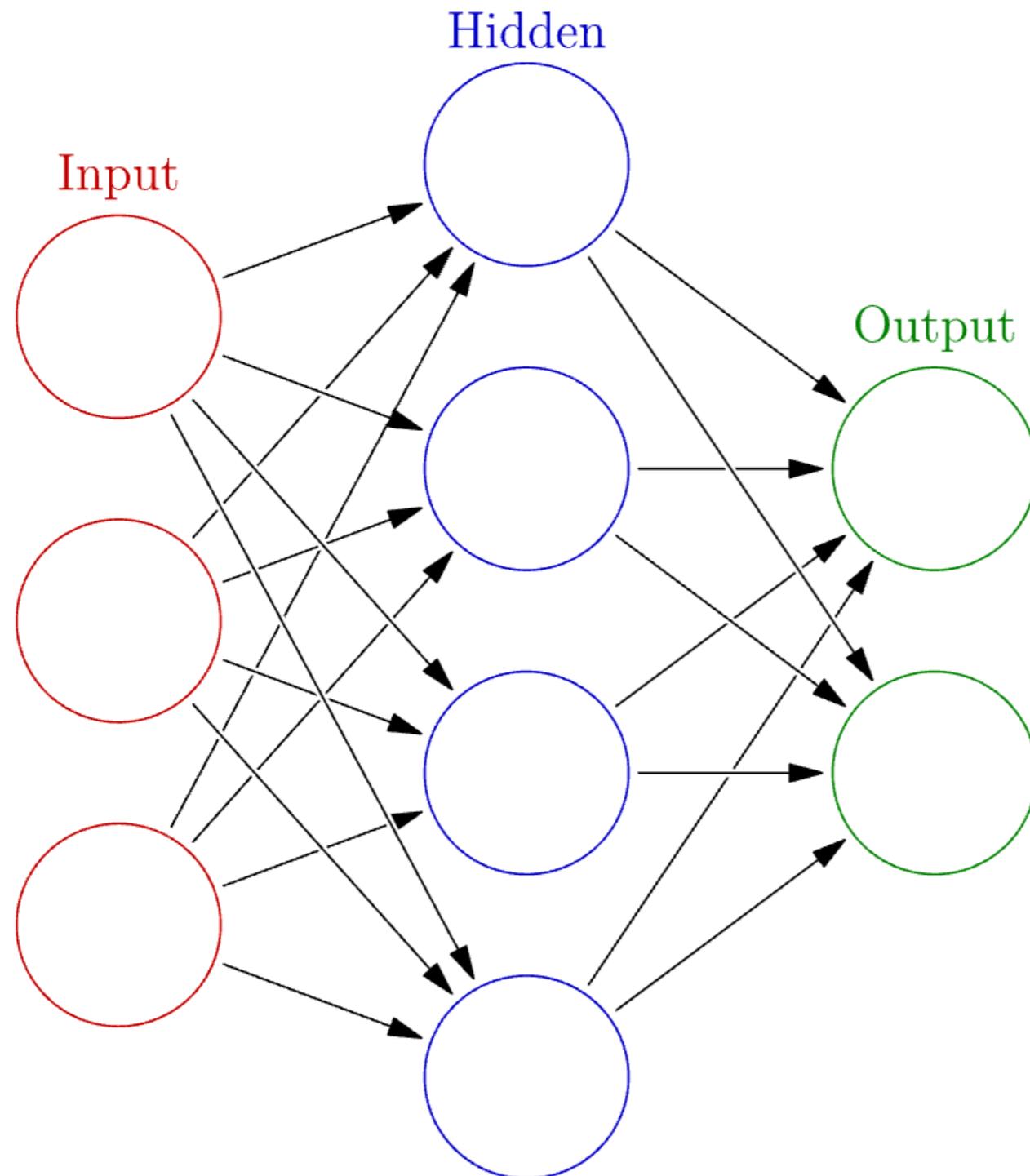
---



- classification based on a large collection of neural units.

# Artificial Neural Networks

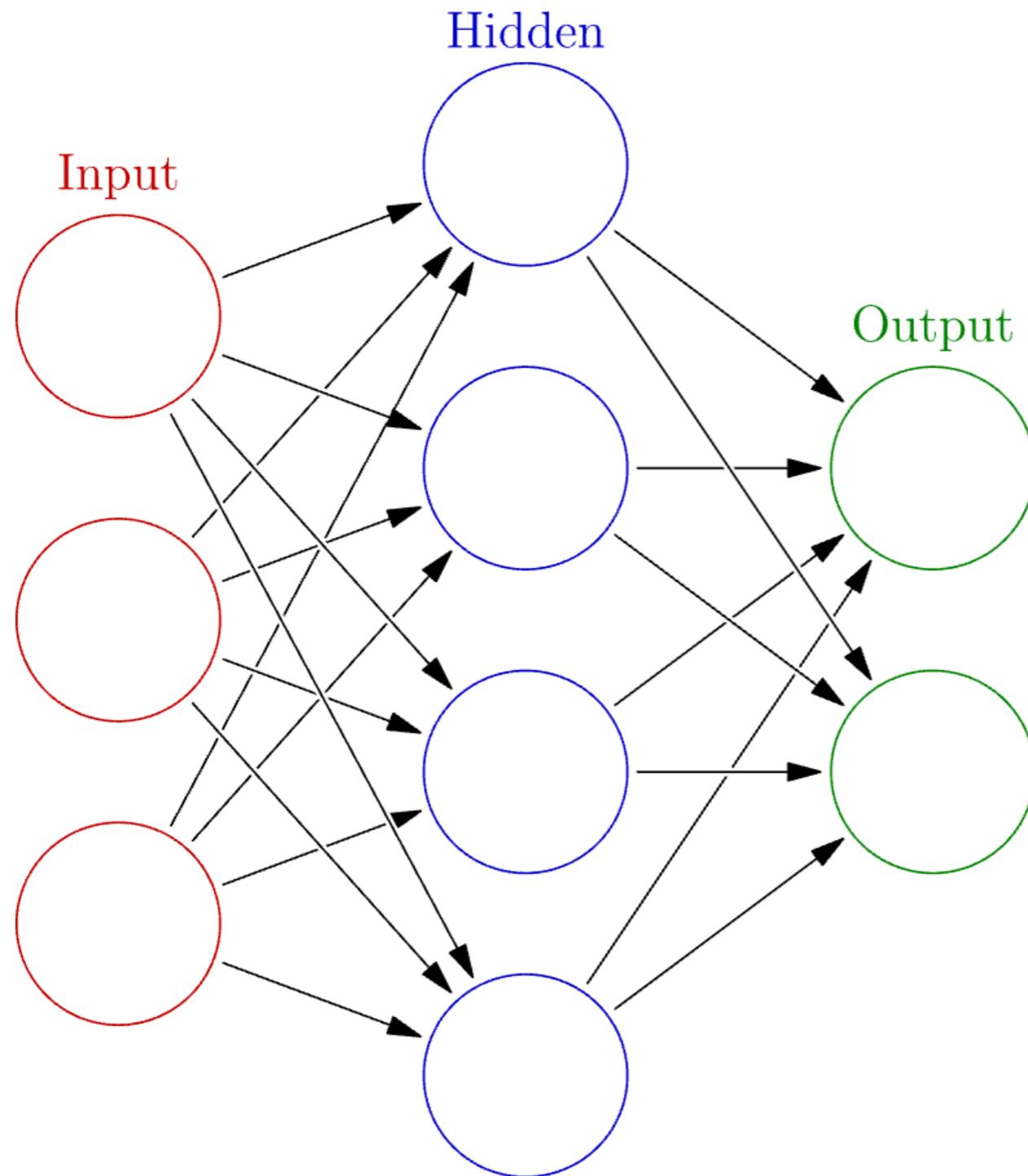
---



- classification based on a large collection of neural units.
- modeling the way a biological brain works.

# Artificial Neural Networks

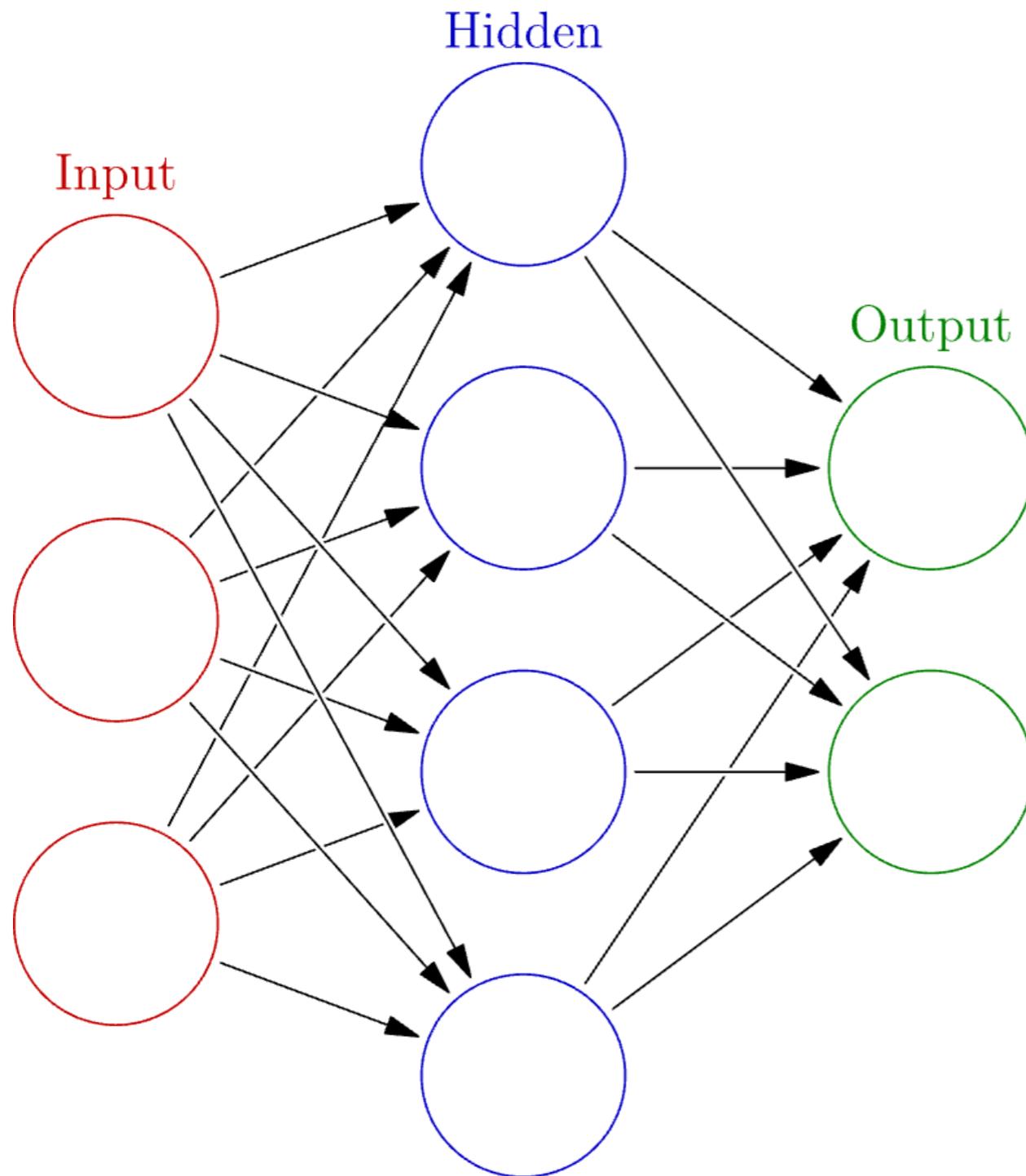
---



- classification based on a large collection of neural units.
- modeling the way a biological brain works.
- Each neural unit is connected with many others.

# Artificial Neural Networks

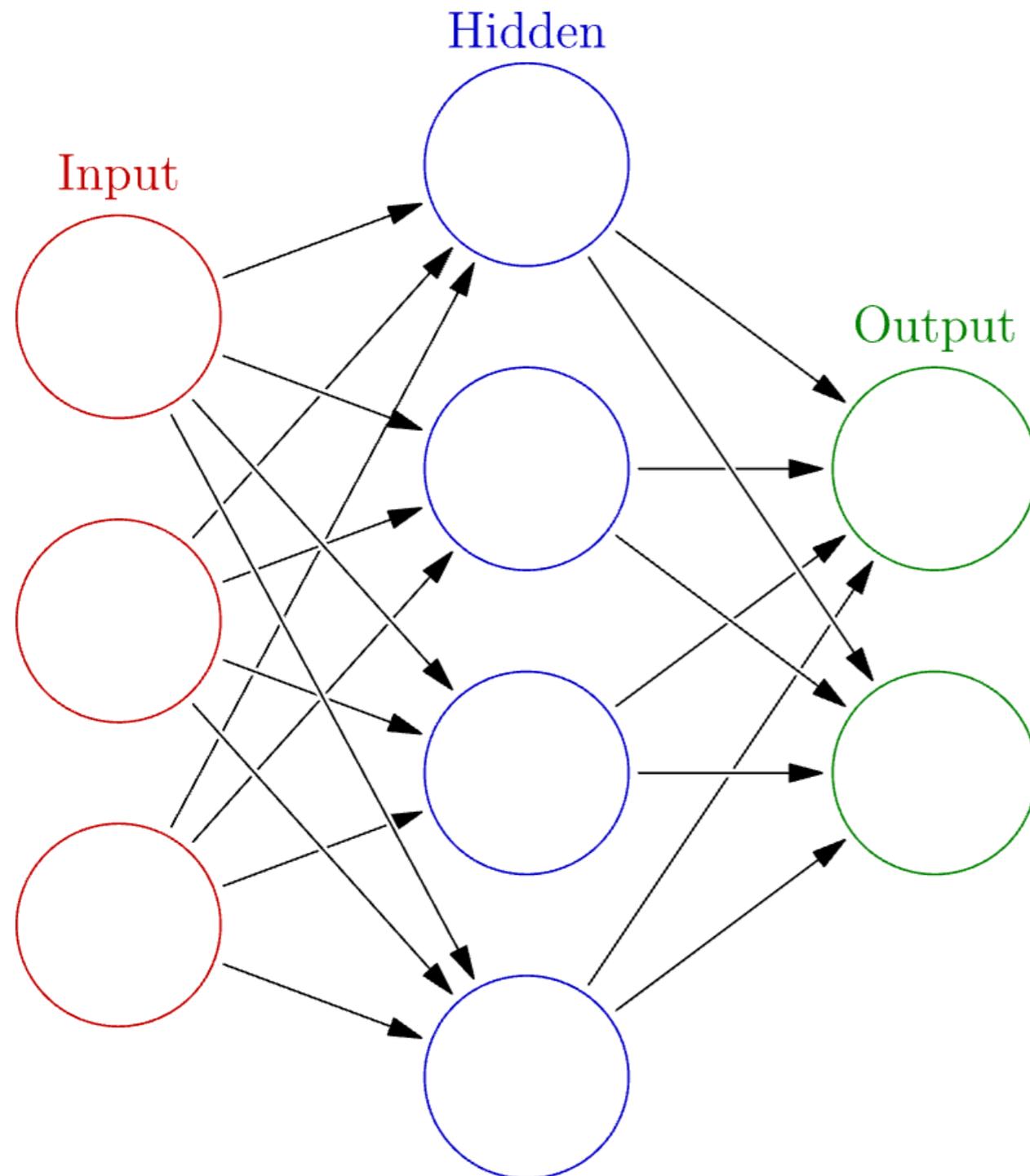
---



- classification based on a large collection of neural units.
- modeling the way a biological brain works.
- Each neural unit is connected with many others.
- links can be enforcing or inhibitory.

# Artificial Neural Networks

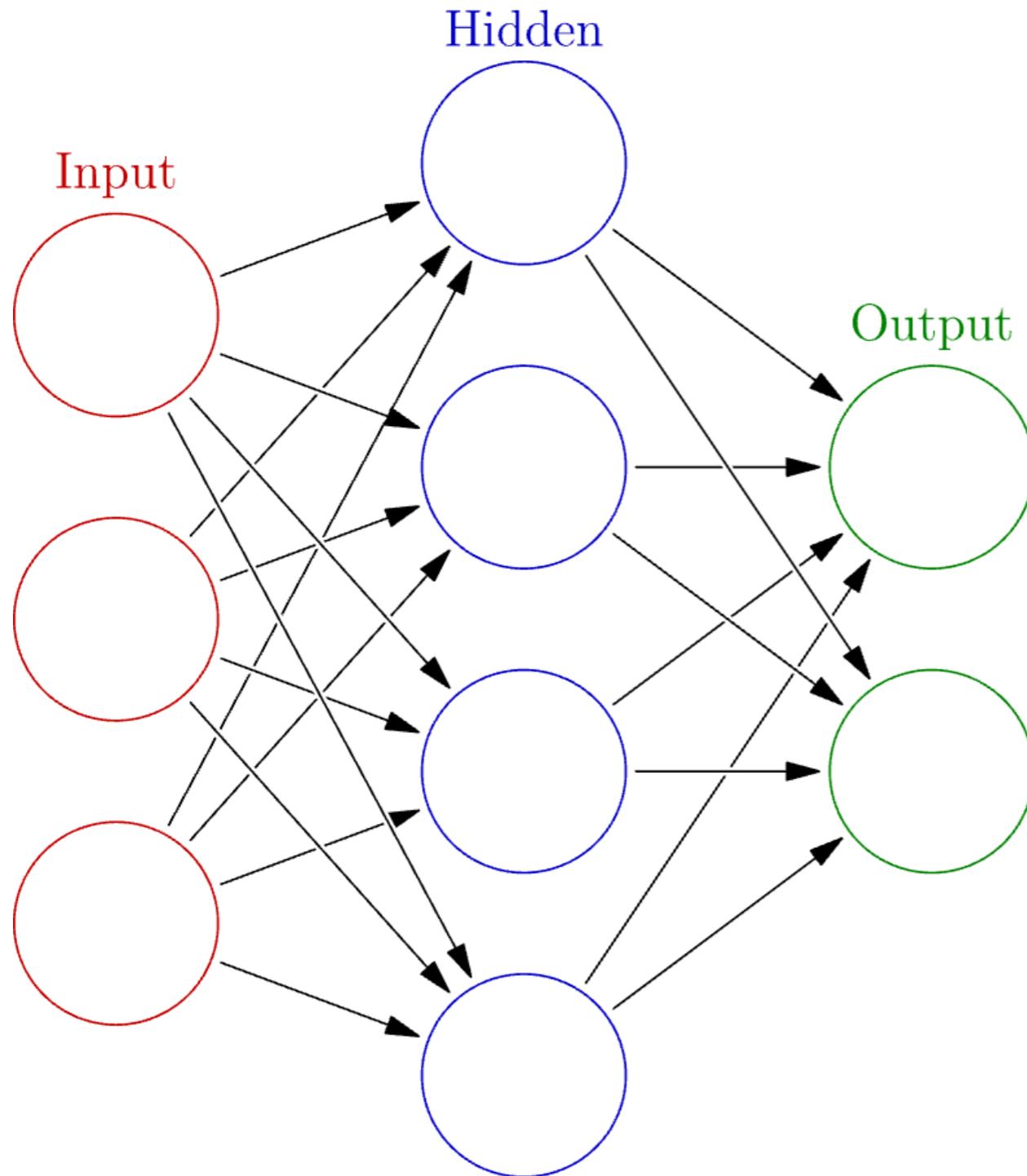
---



- classification based on a large collection of neural units.
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- Each neural unit is connected with many others.
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- Each individual neural unit has a summation function.

# Artificial Neural Networks

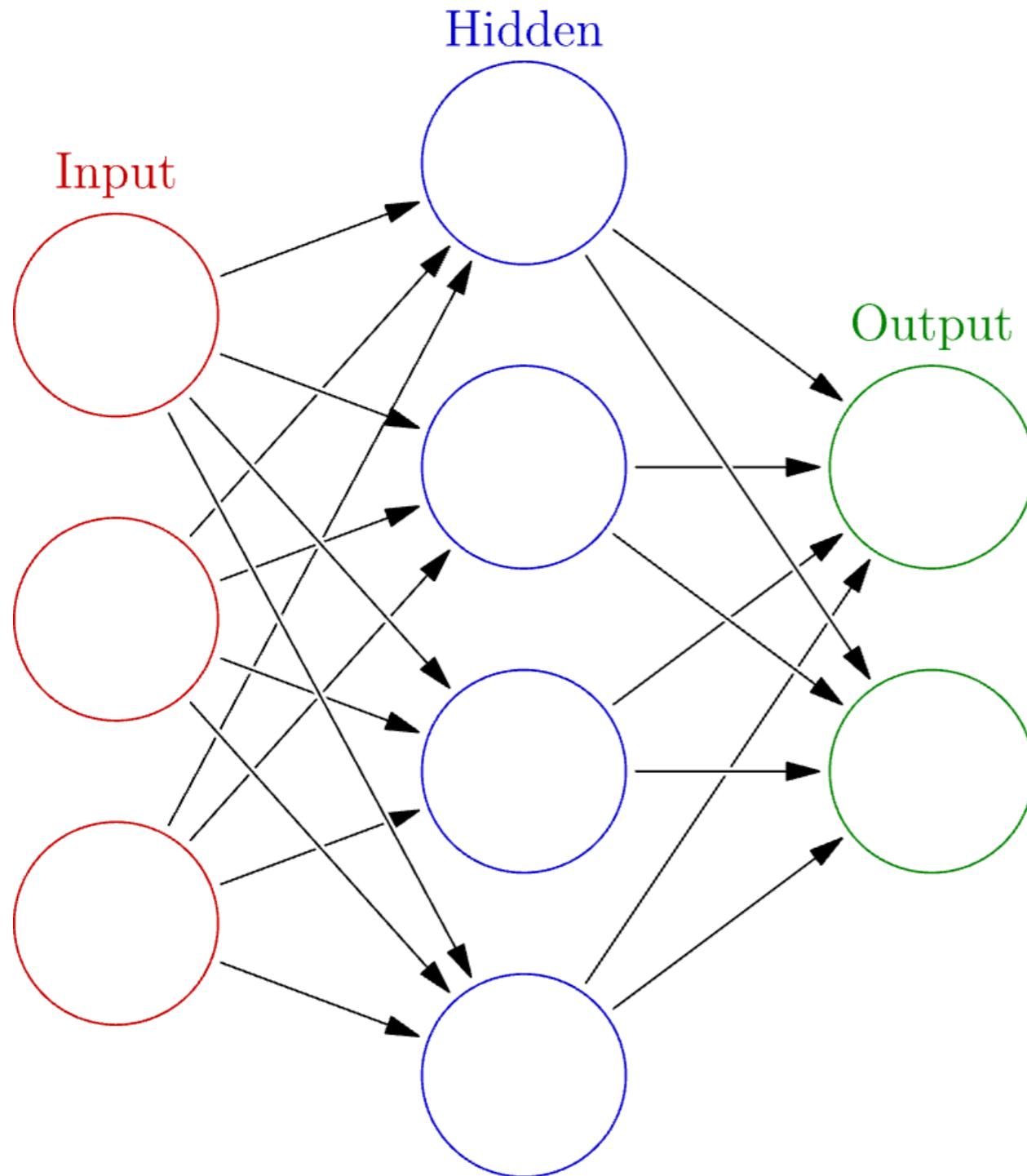
---



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- These systems are self-learning and trained.

# Artificial Neural Networks

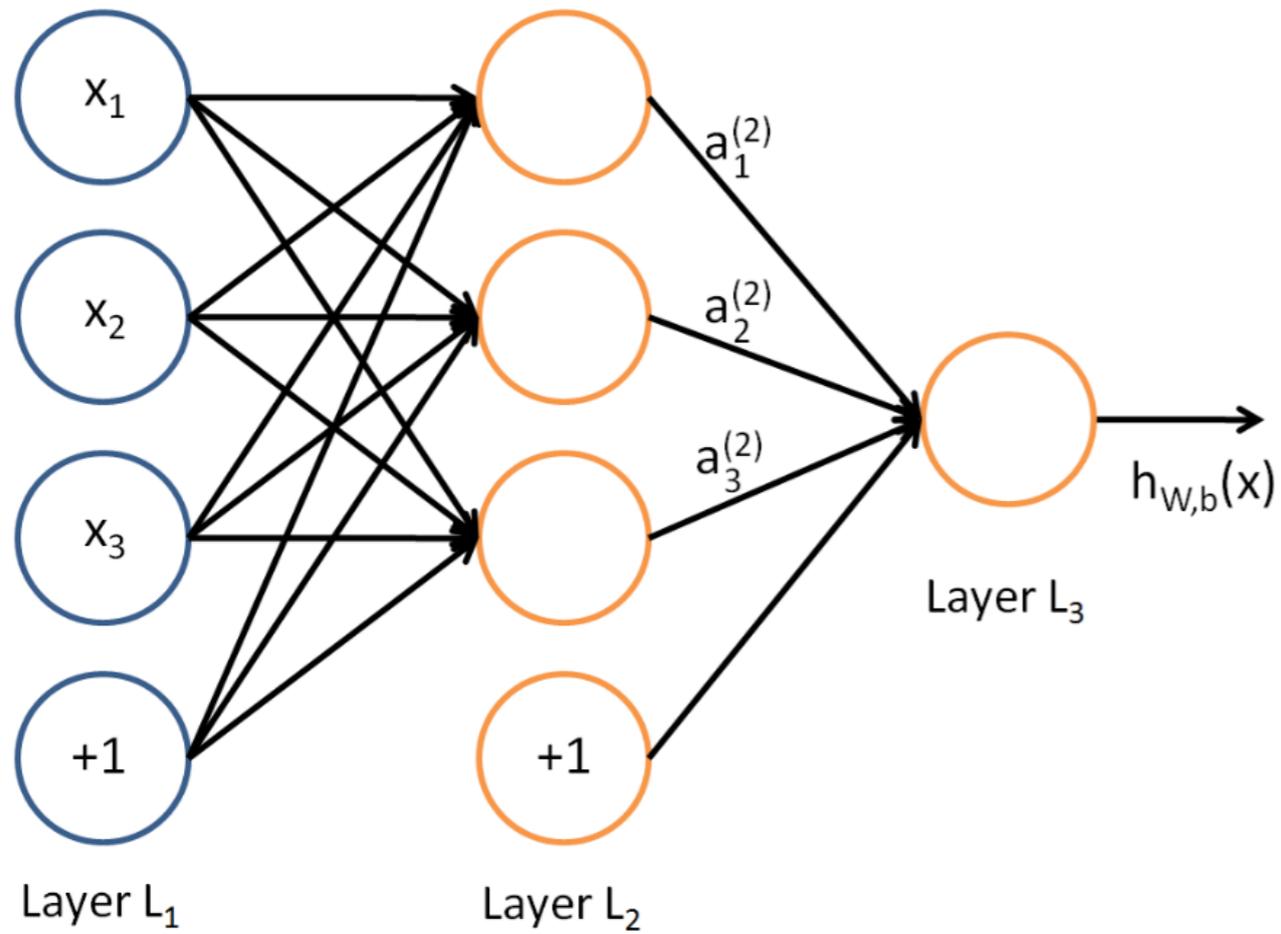
---



- classification based on a large collection of neural units.
- modeling the way a biological brain works.
- Each neural unit is connected with many others.
- links can be enforcing or inhibitory.
- Each individual neural unit has a summation function.
- These systems are self-learning and trained.
- There can be multiple layers.

# Artificial Neural Networks

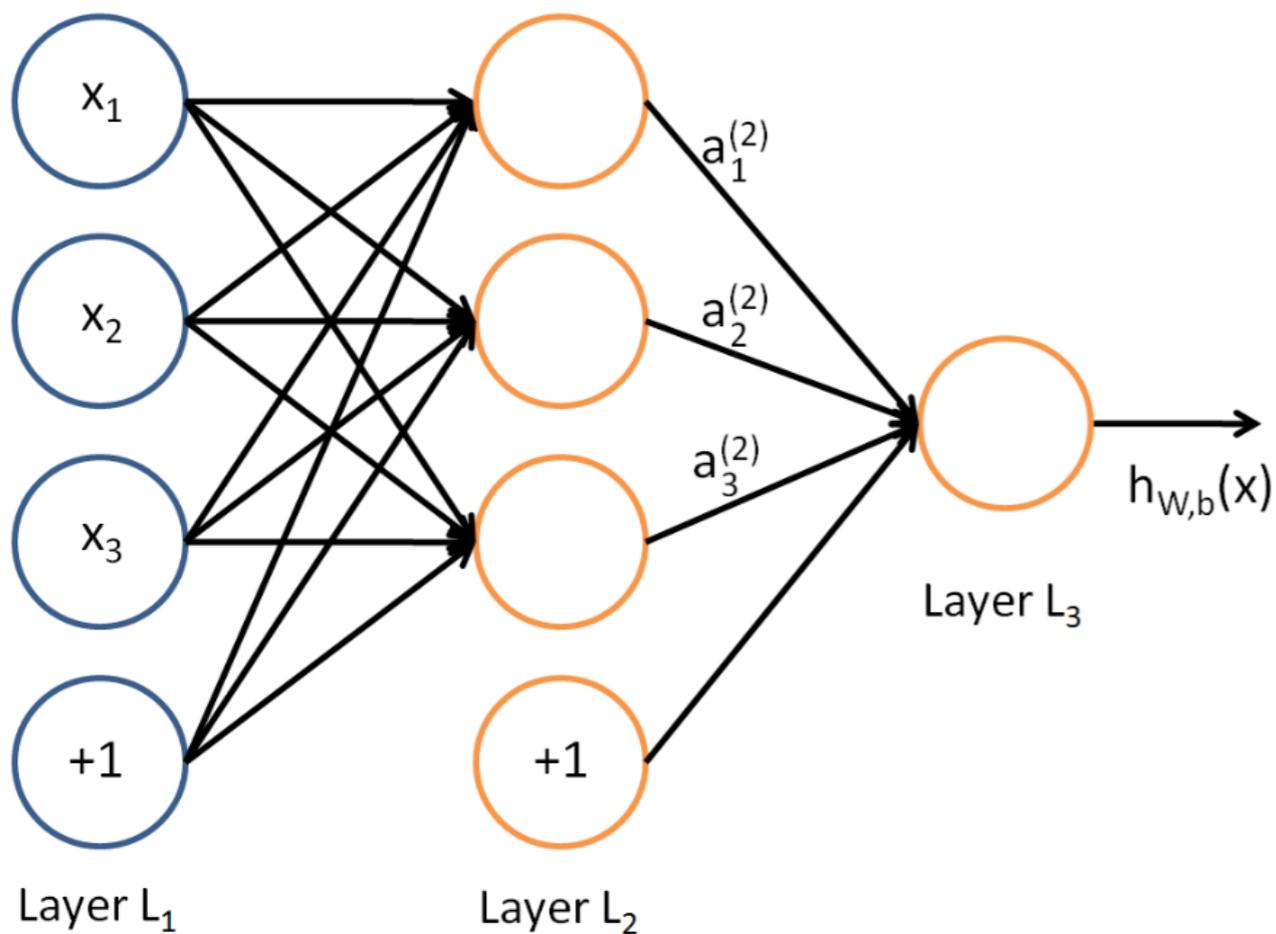
---



# Artificial Neural Networks

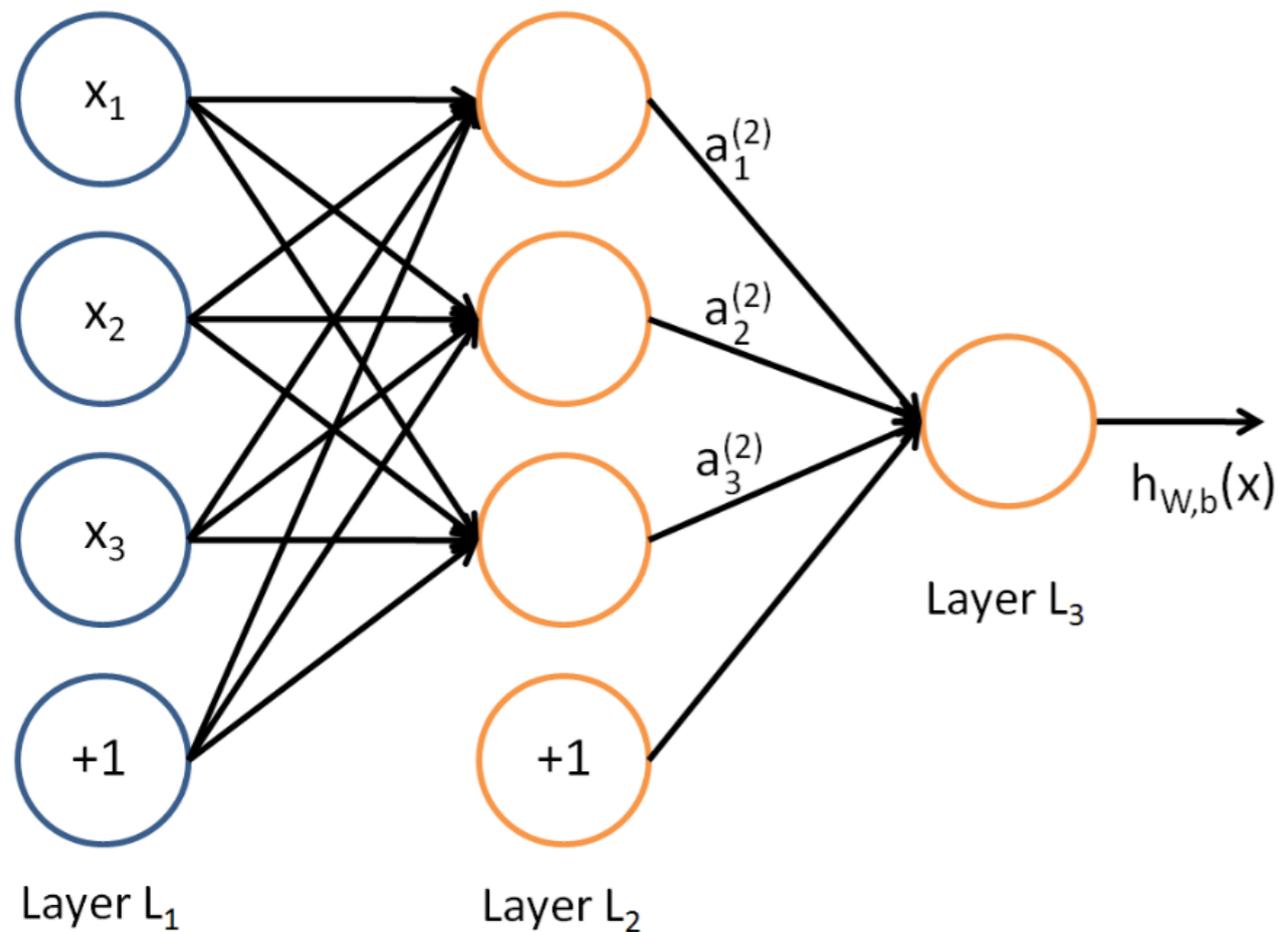
---

- Orange circles represent neurons.



# Artificial Neural Networks

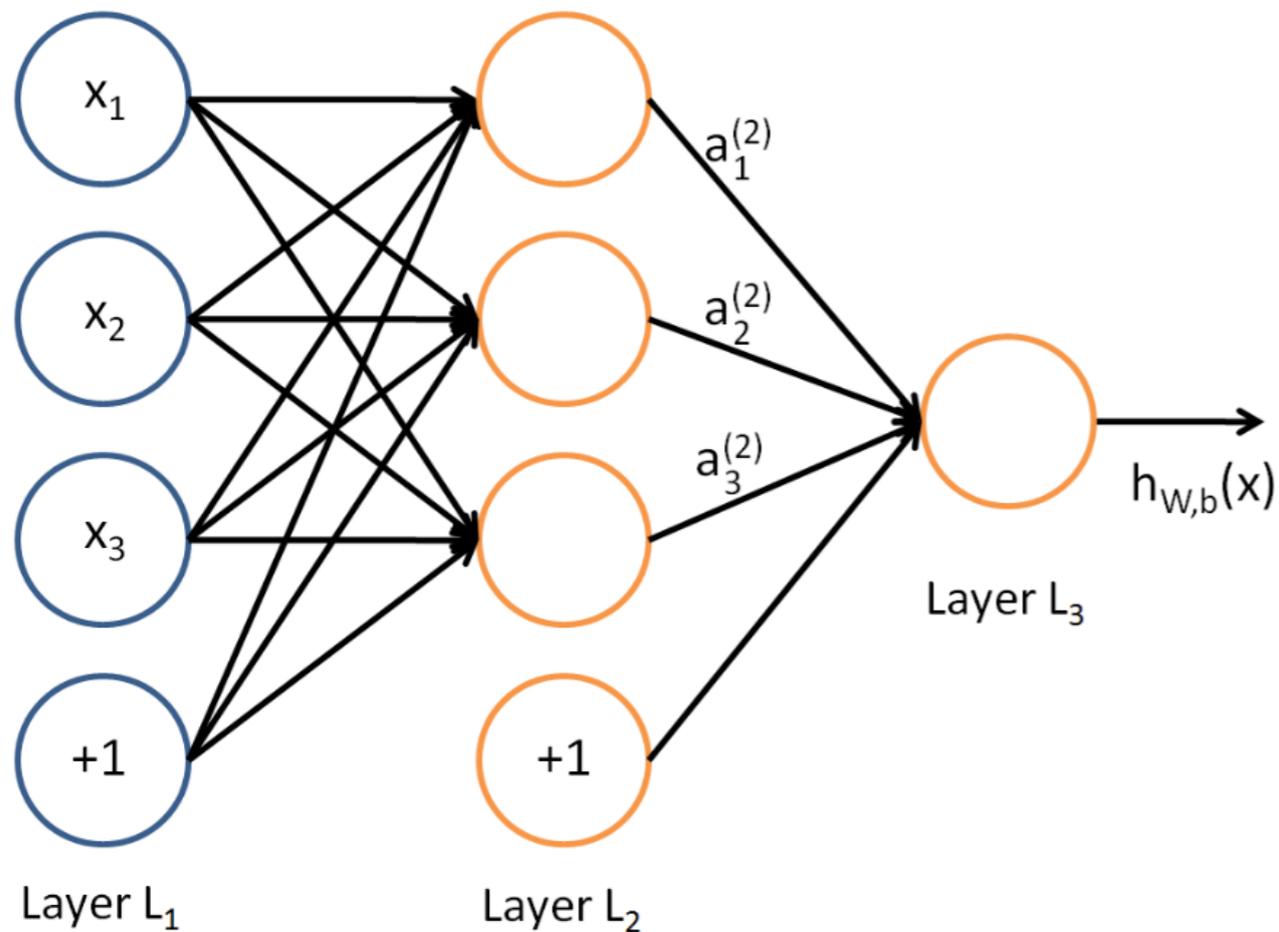
---



- Orange circles represent neurons.
- A neuron can be the input of another.

# Artificial Neural Networks

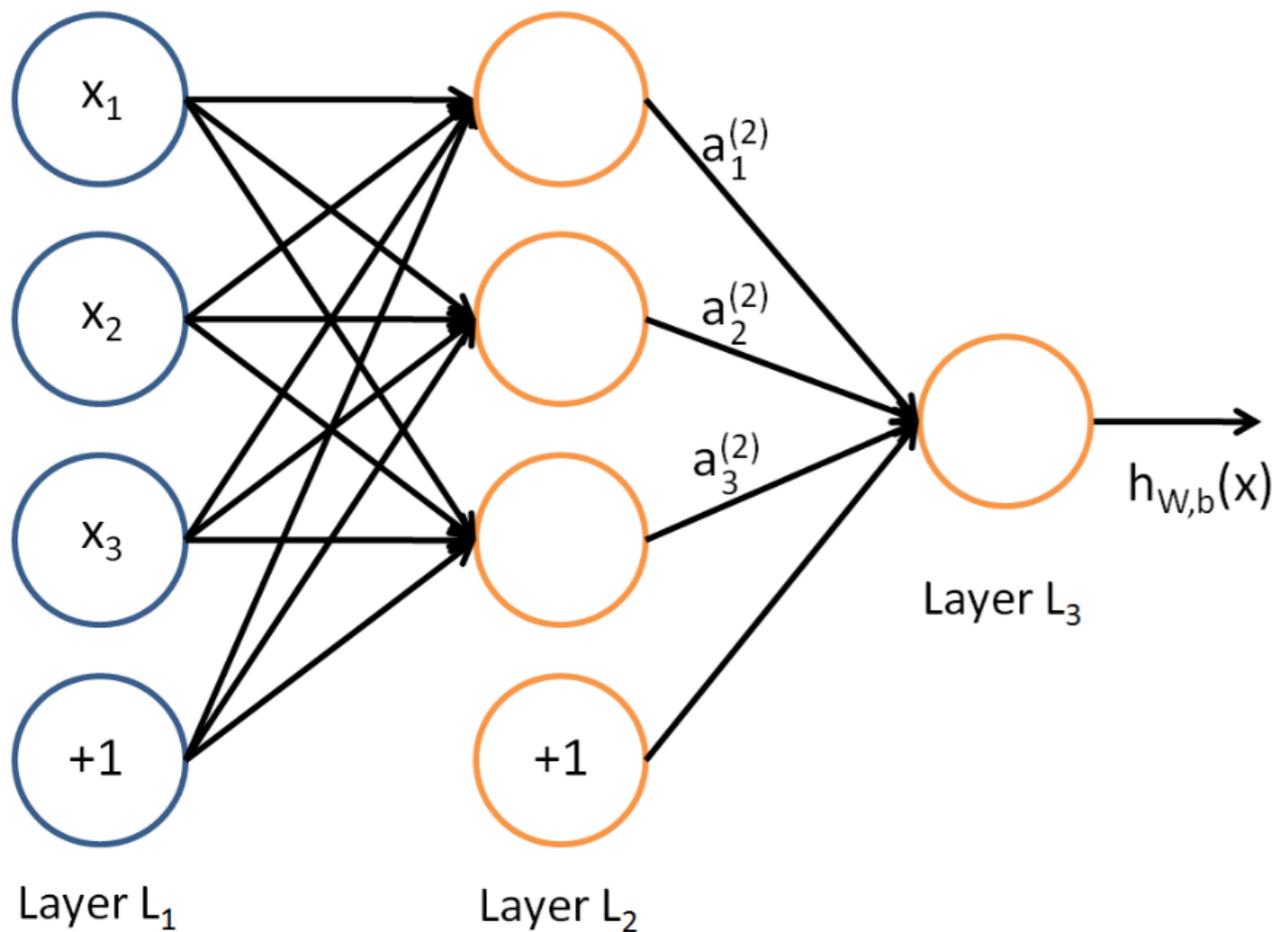
---



- Orange circles represent neurons.
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- $x_1$ ,  $x_2$ , and  $x_3$  in L<sub>1</sub> are the inputs.

# Artificial Neural Networks

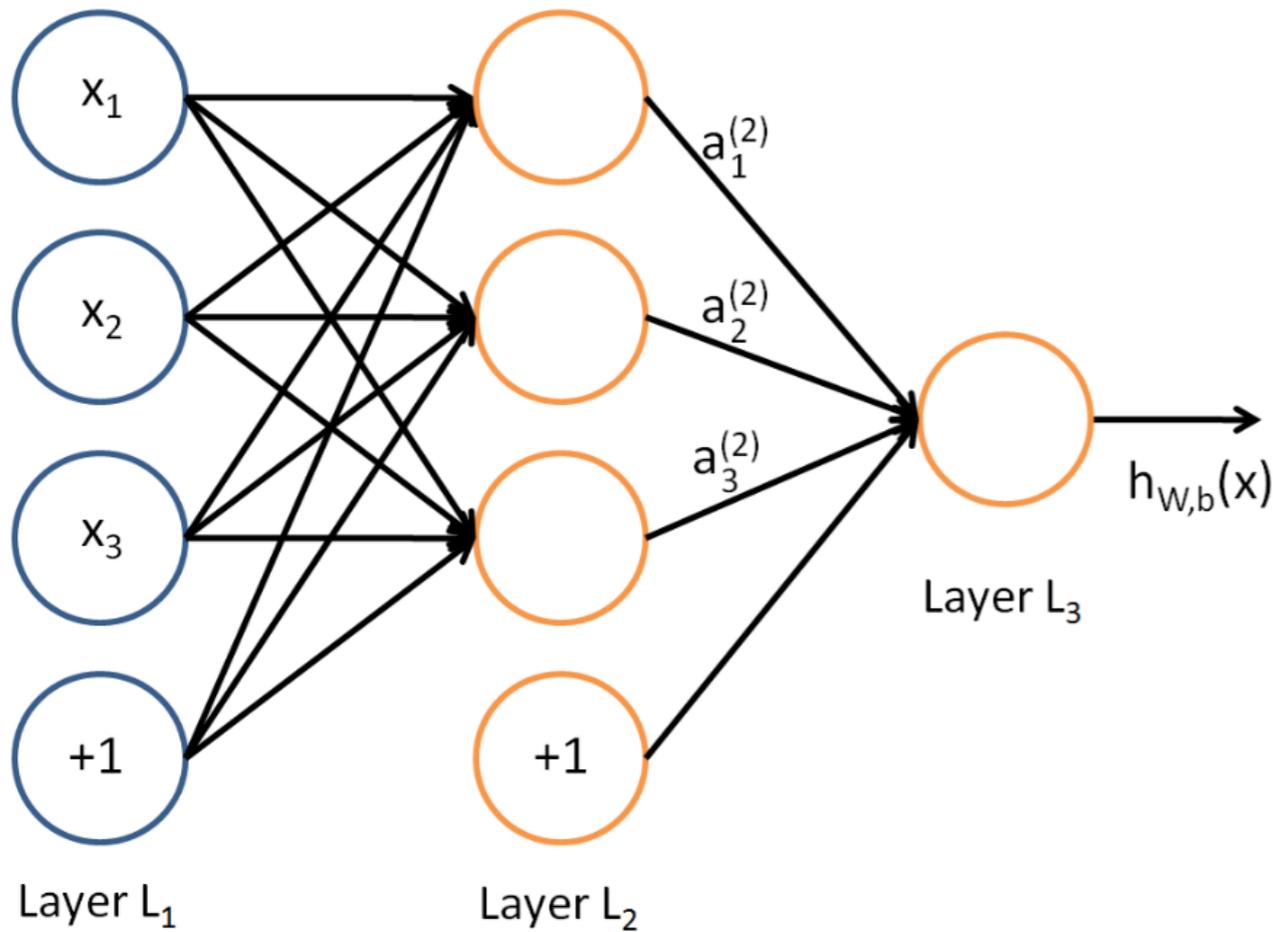
---



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- “+1” are called bias units.

# Artificial Neural Networks

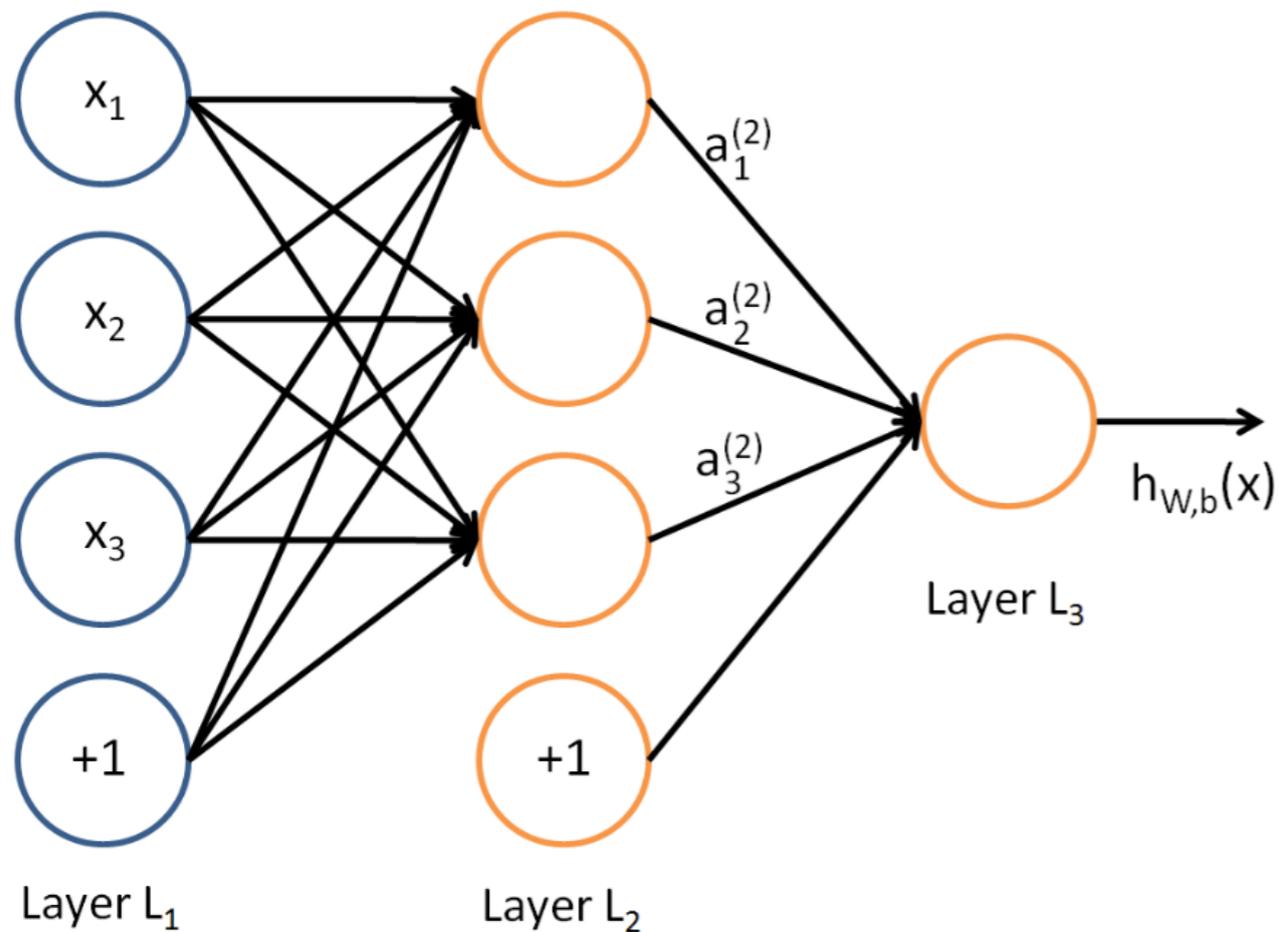
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- $L_2$  is called a hidden layer.

# Artificial Neural Networks

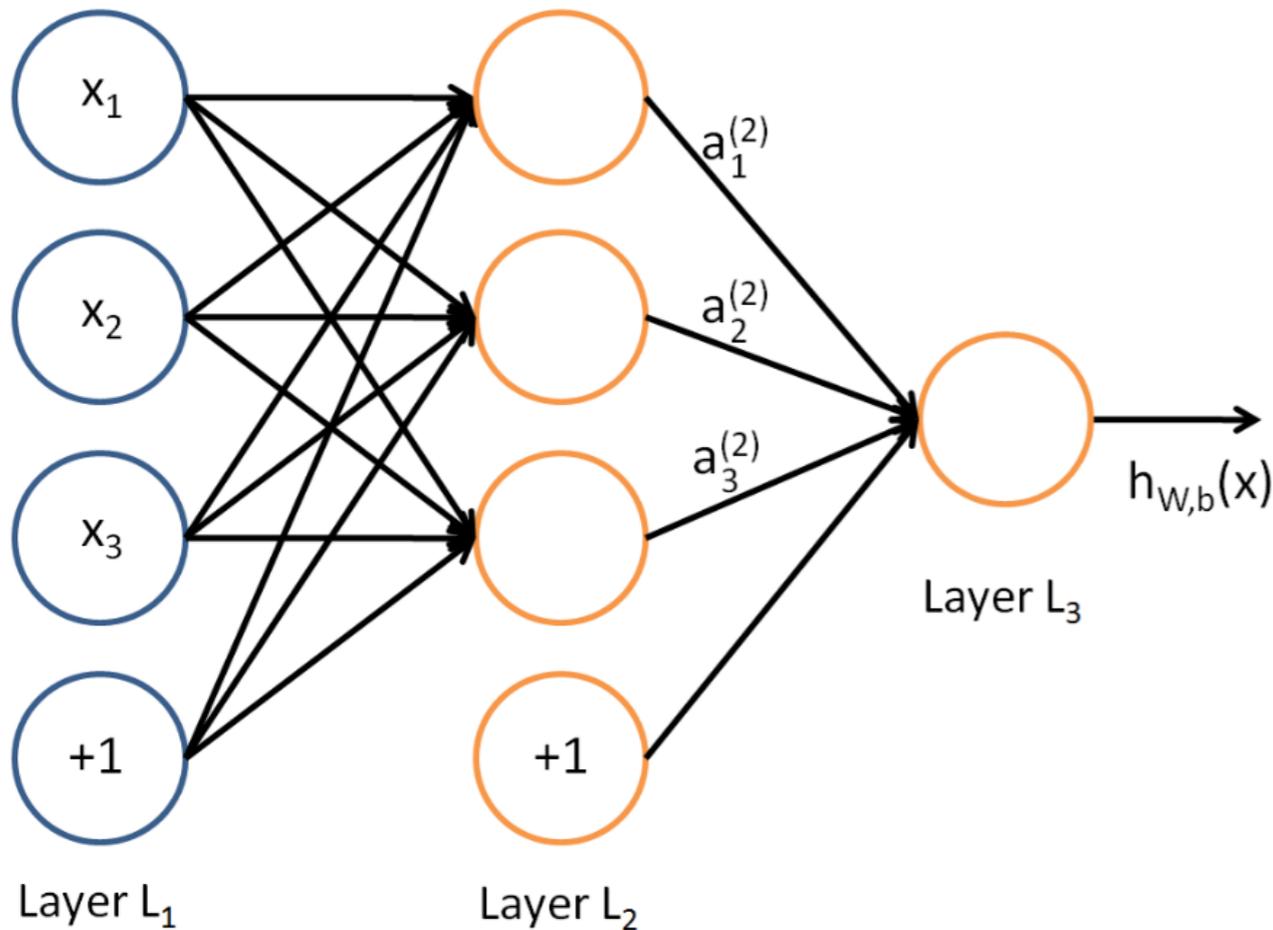
---



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# Artificial Neural Networks

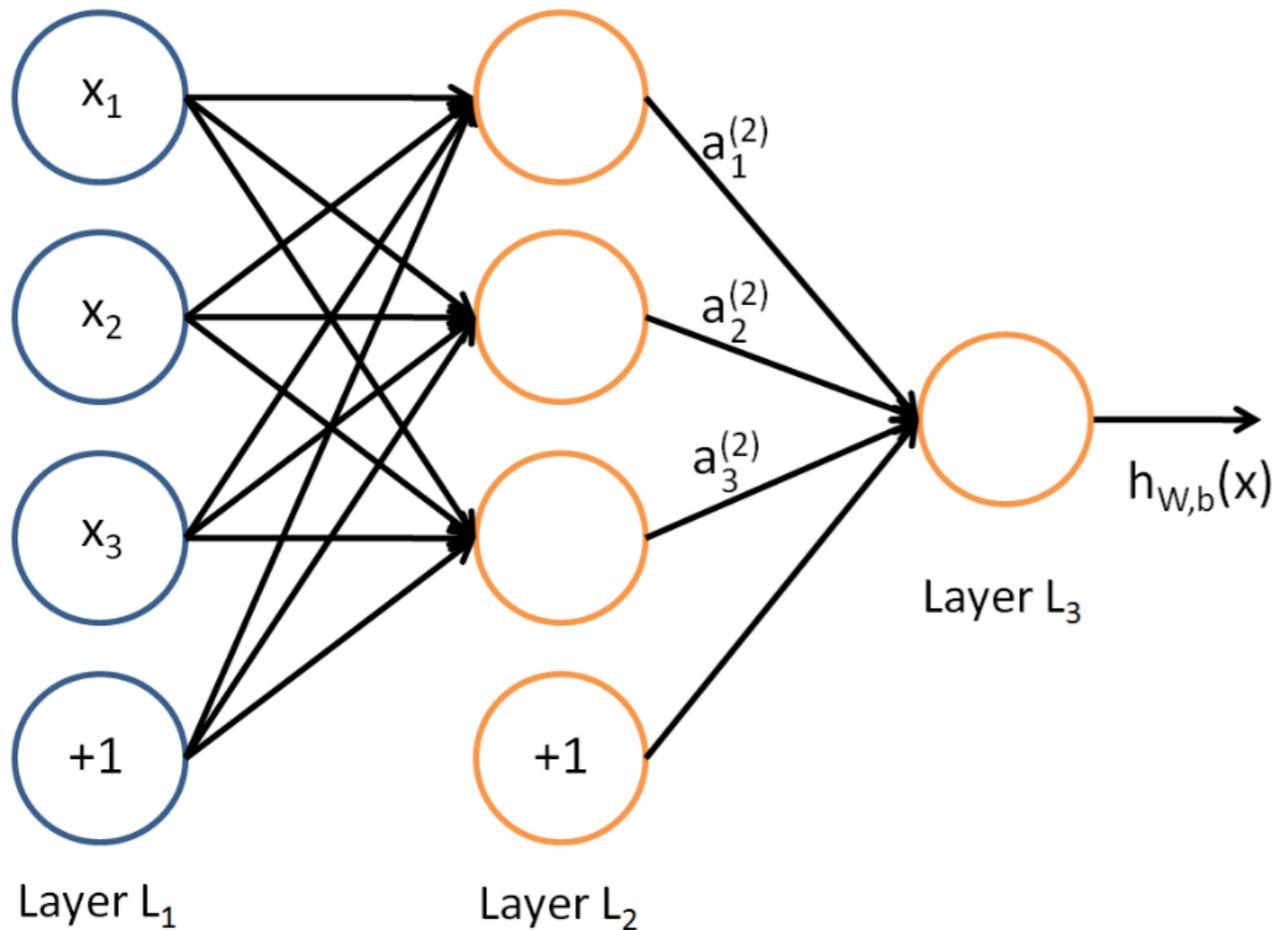
---



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- $L_3$  is the output layer.
- This ANN has 3 input units and 1 output unit.

# Artificial Neural Networks

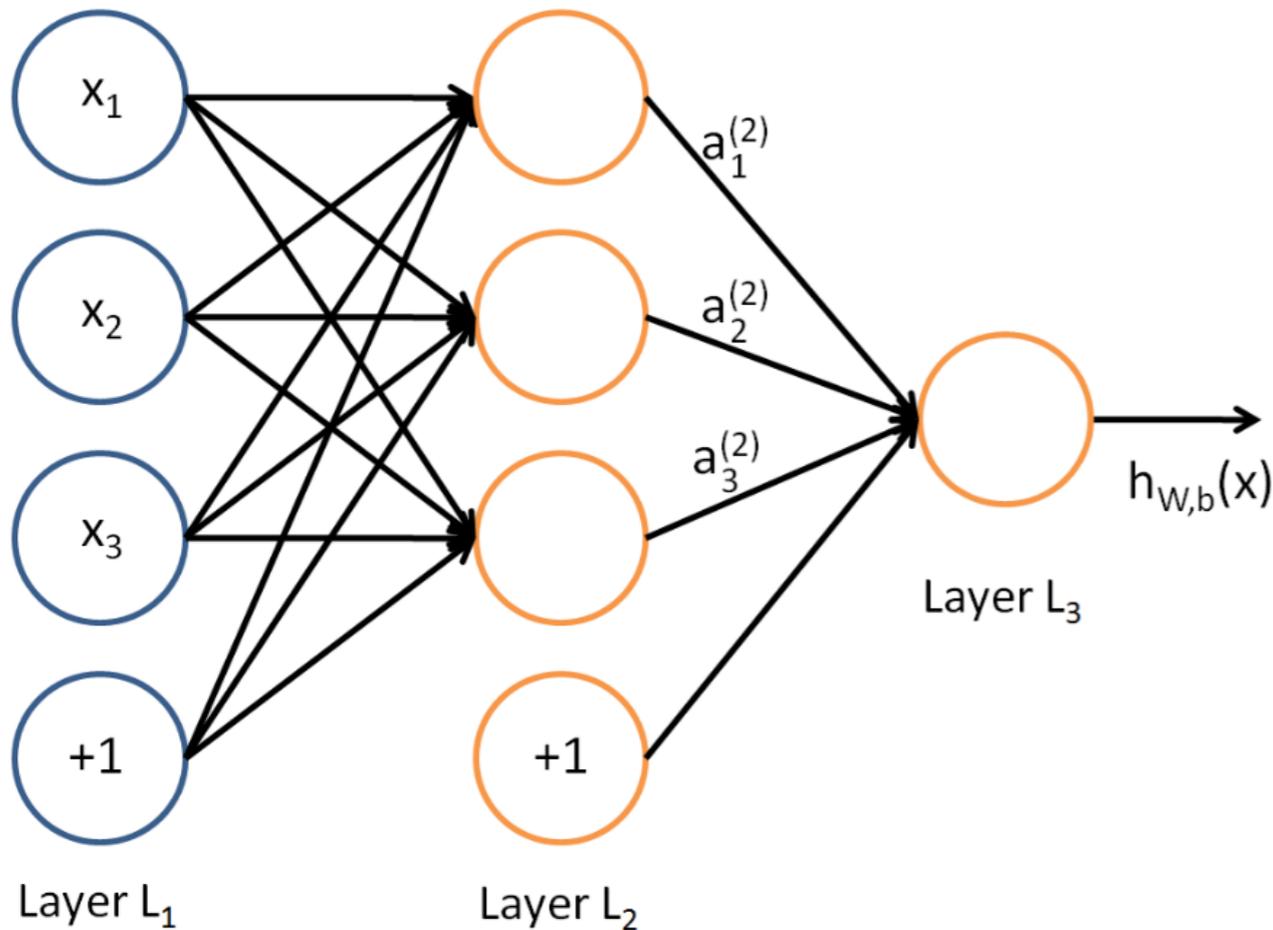
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- Each neuron in  $L_2$  is a computational unit and outputs  $h = f(W_1x_1 + W_2x_2 + W_3x_3 + b)$

# Artificial Neural Networks

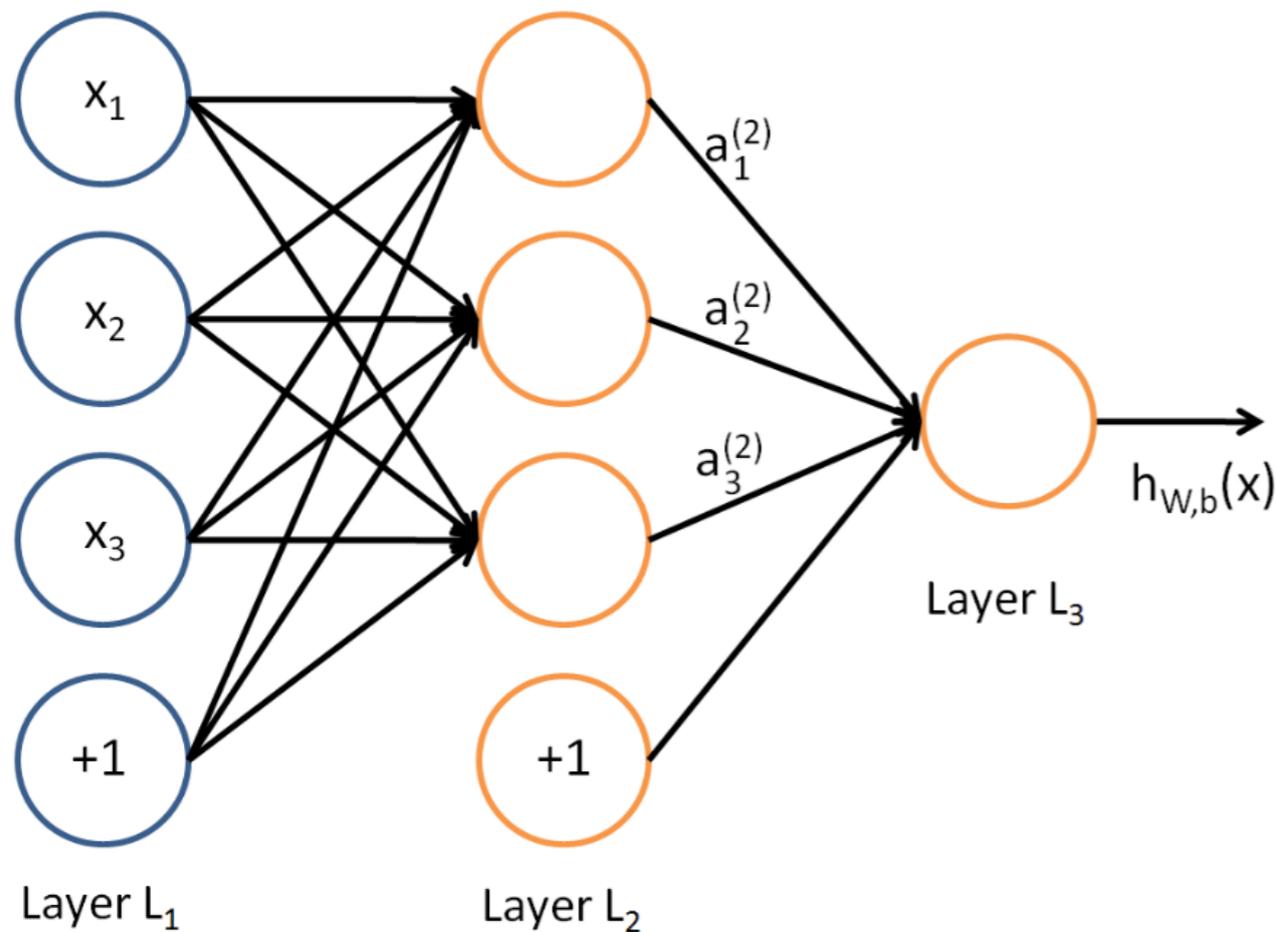
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- $h$  is called activation function and we choose  $f(z) = 1/(1 + e^{-z})$

# Artificial Neural Networks

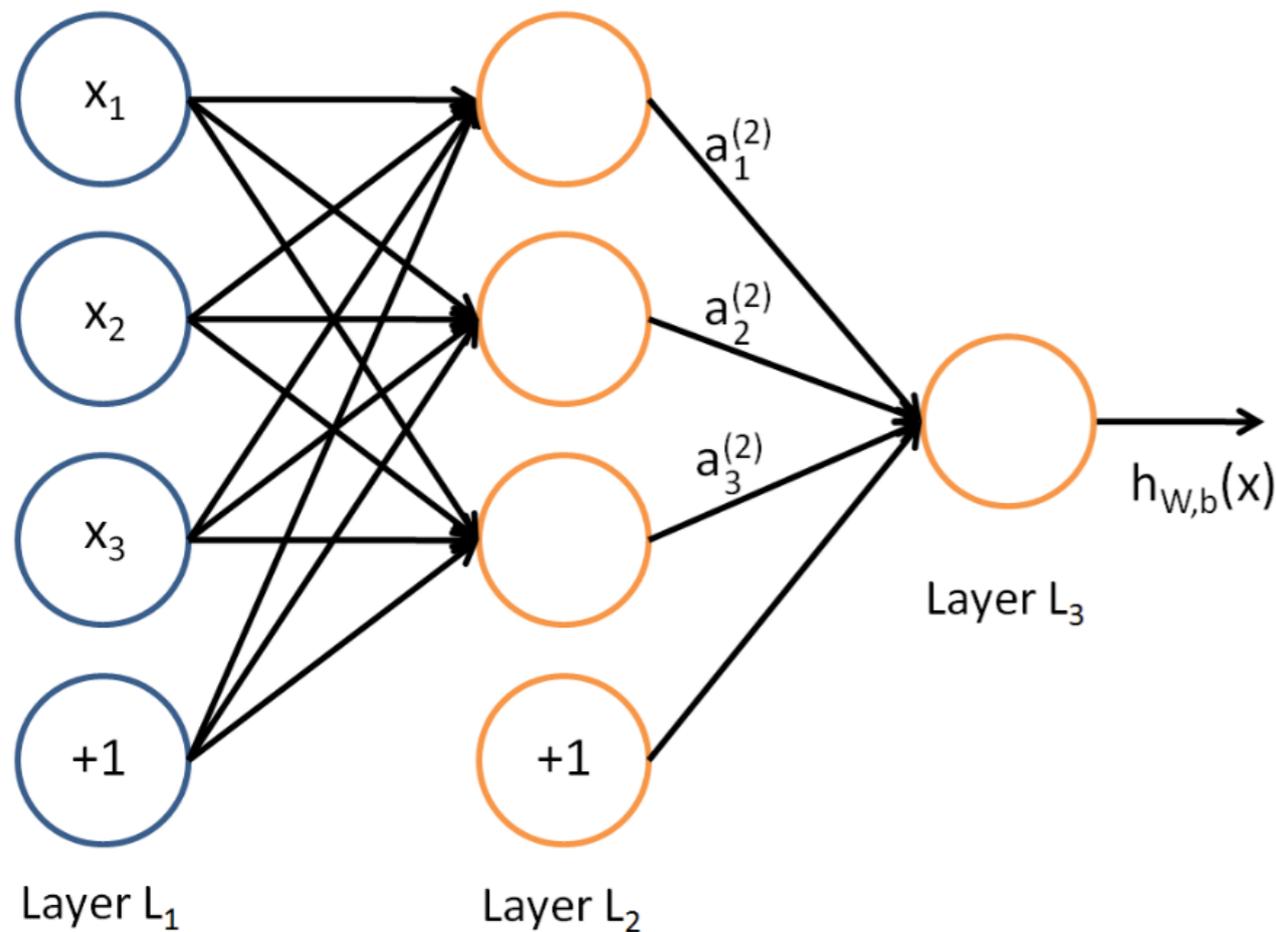
---



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- $W$  is the weight and varies path-by-path.

# Artificial Neural Networks

---

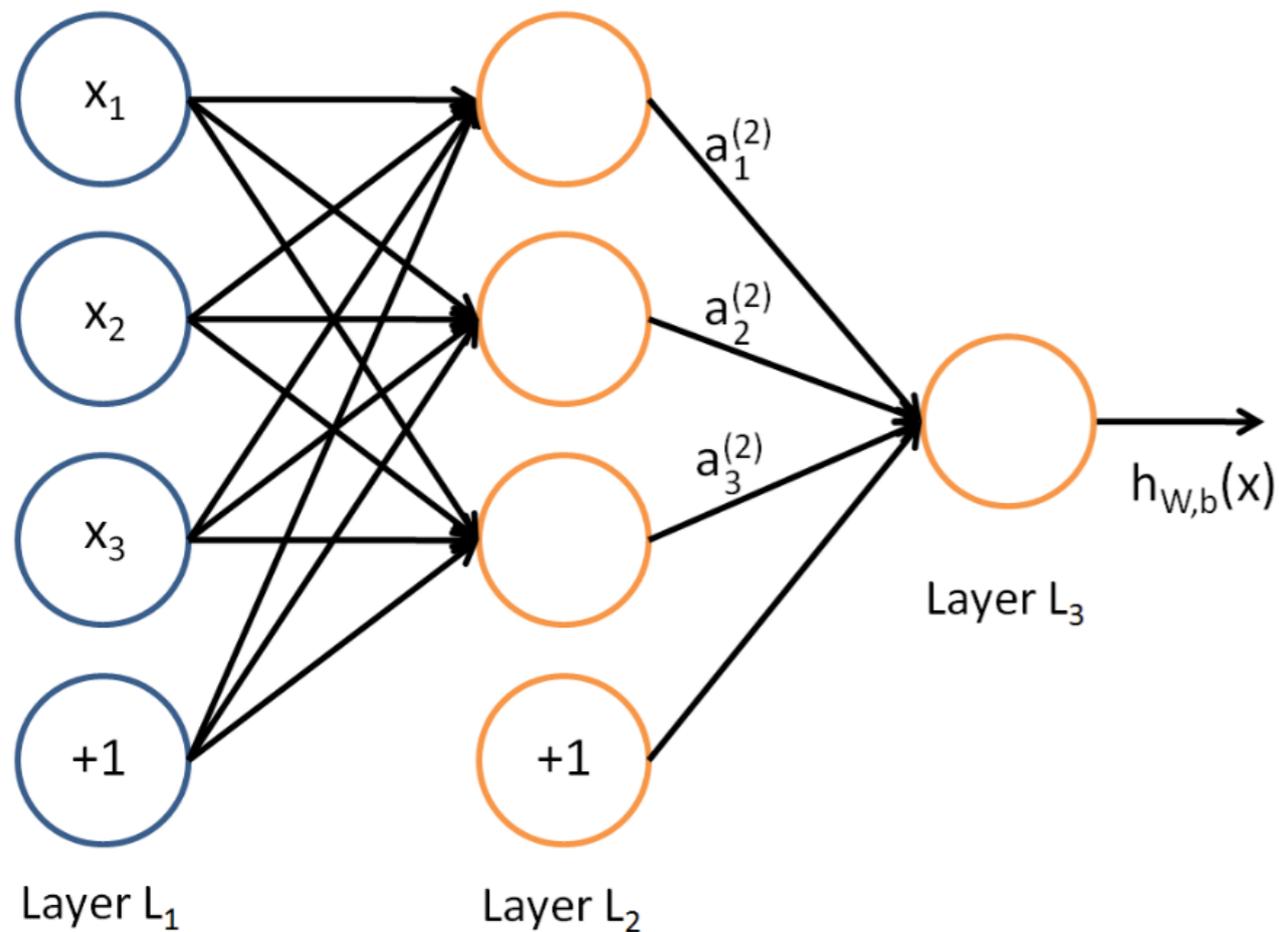


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# Artificial Neural Networks

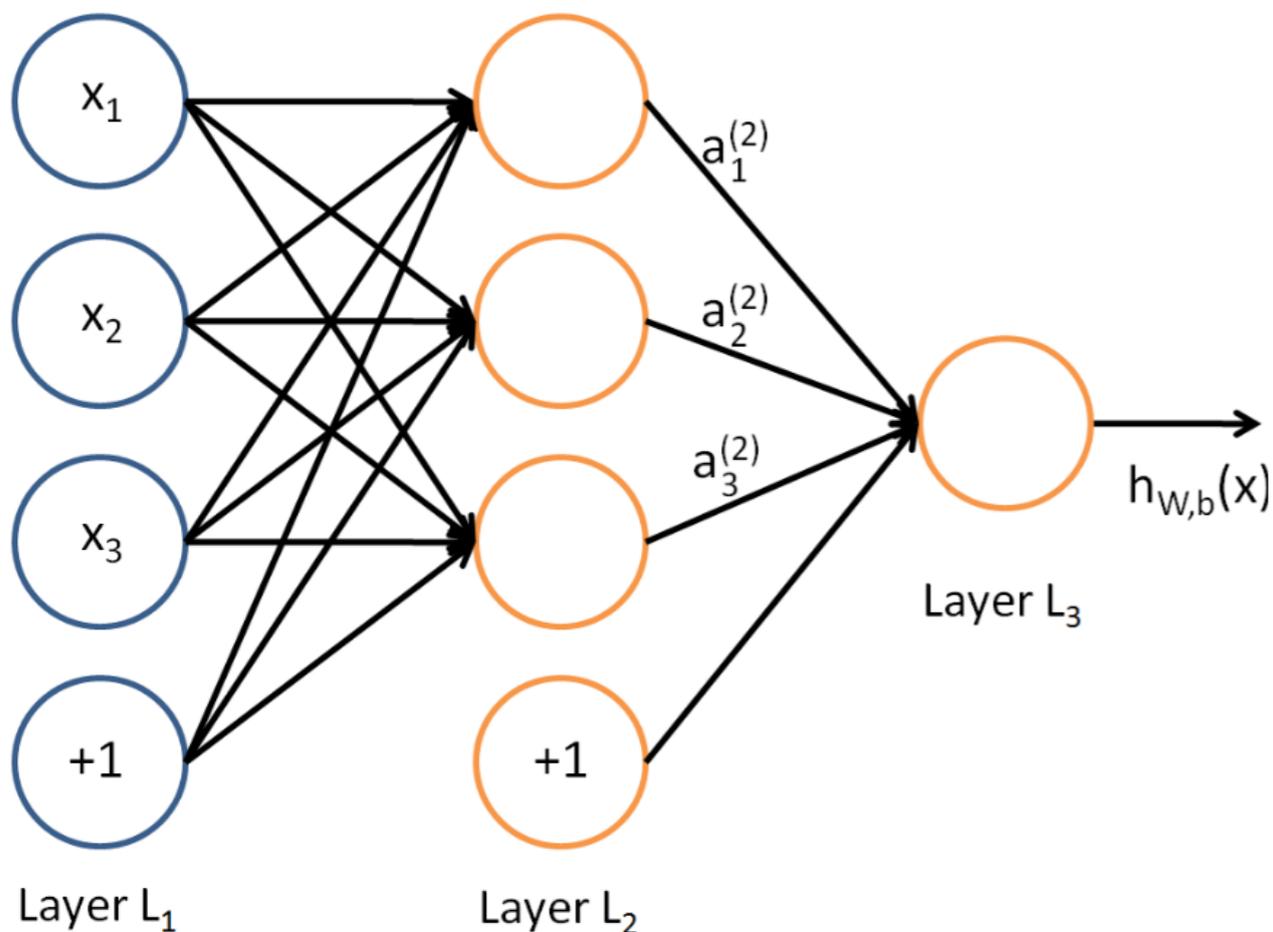
---

We can express these functions by the following equations.



# Artificial Neural Networks

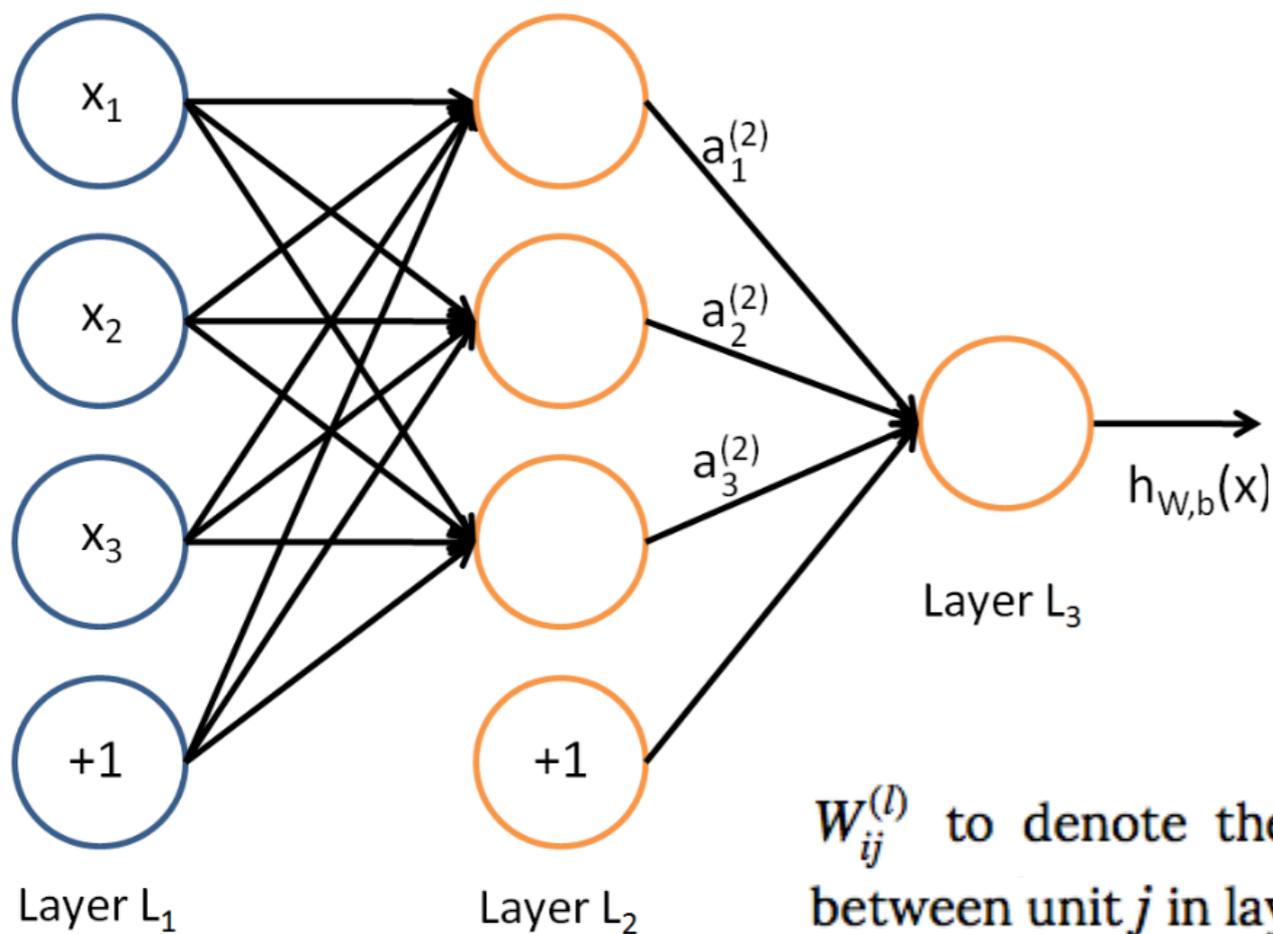
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# Artificial Neural Networks

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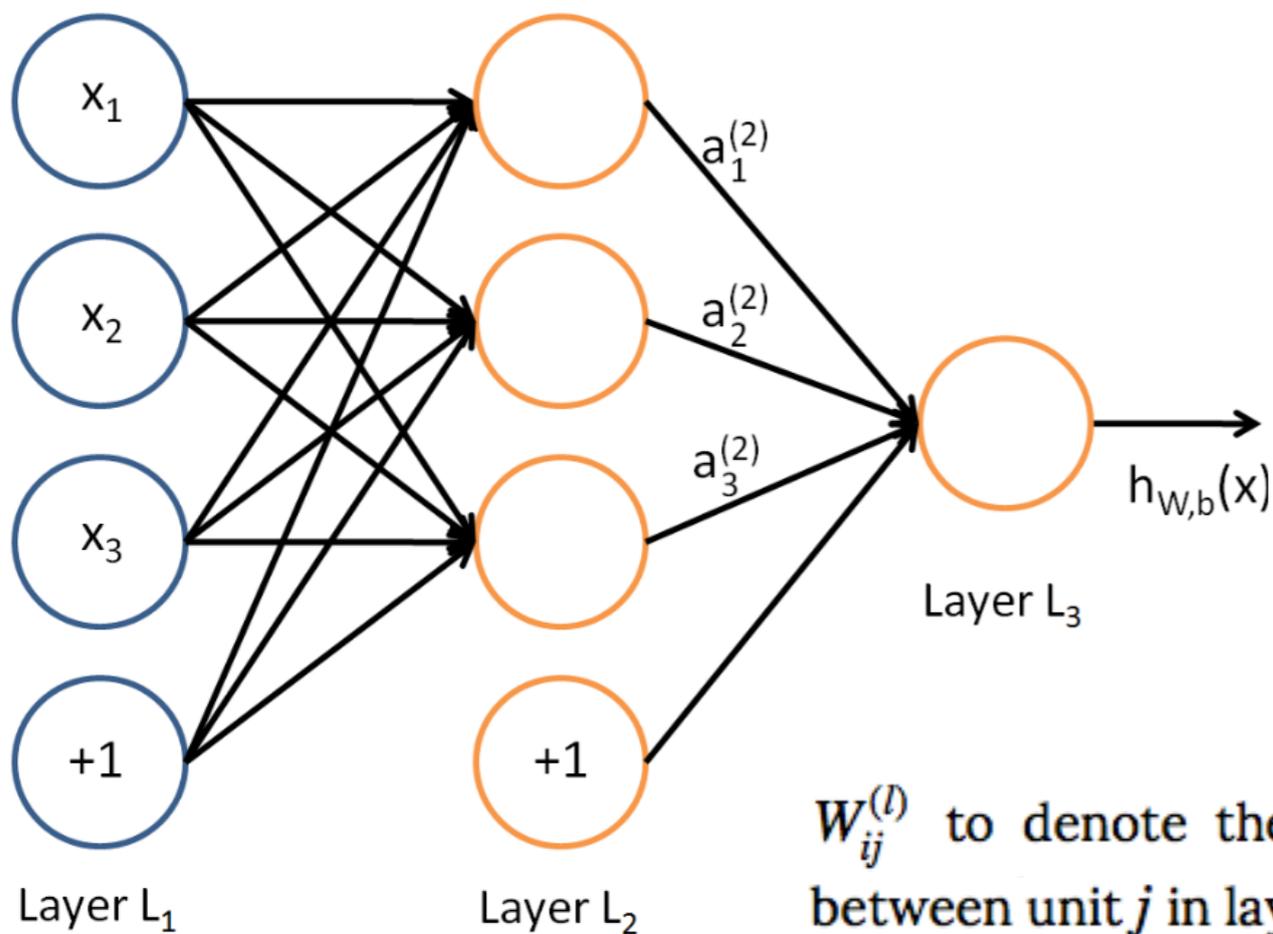


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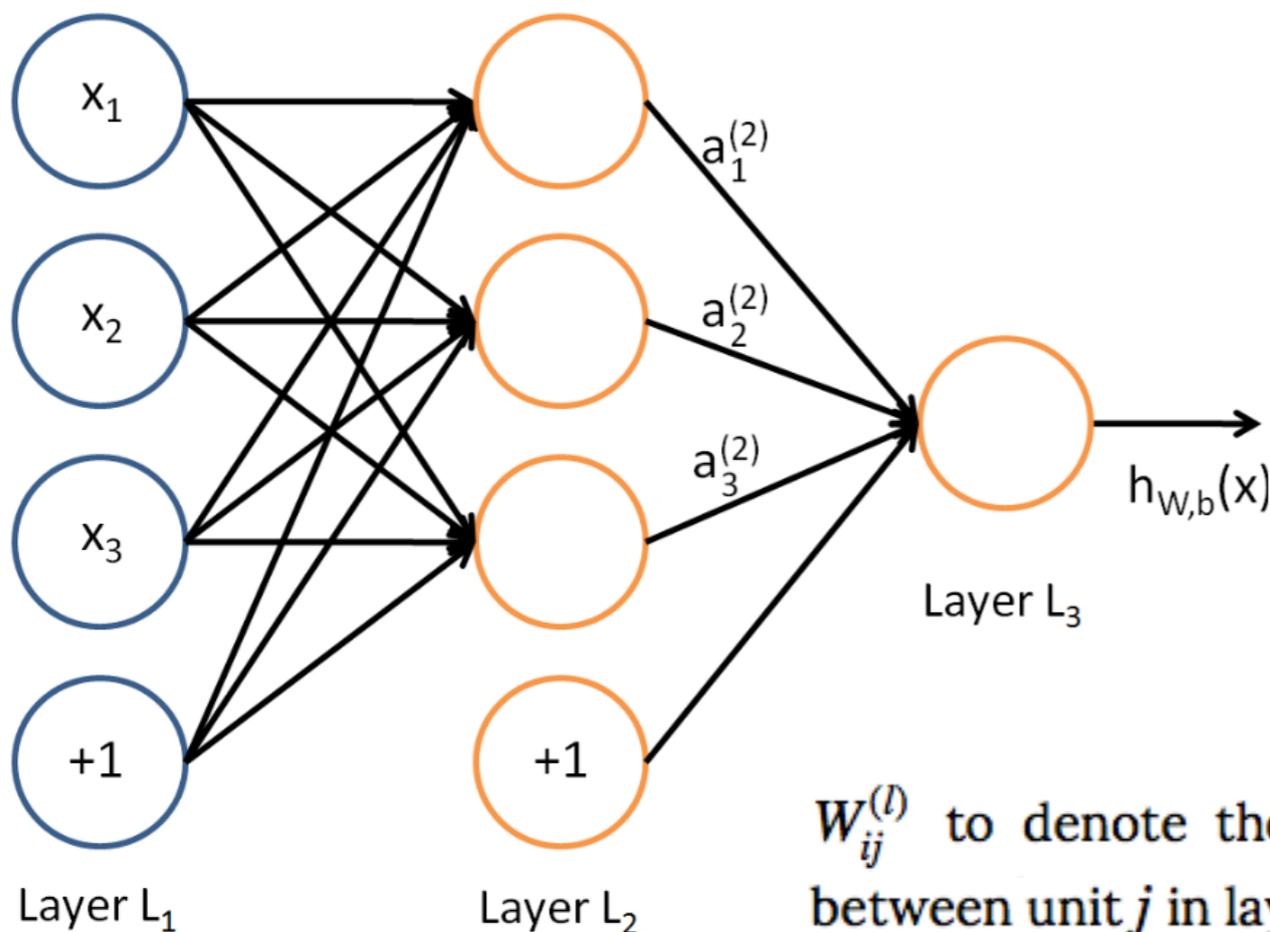
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# Artificial Neural Networks

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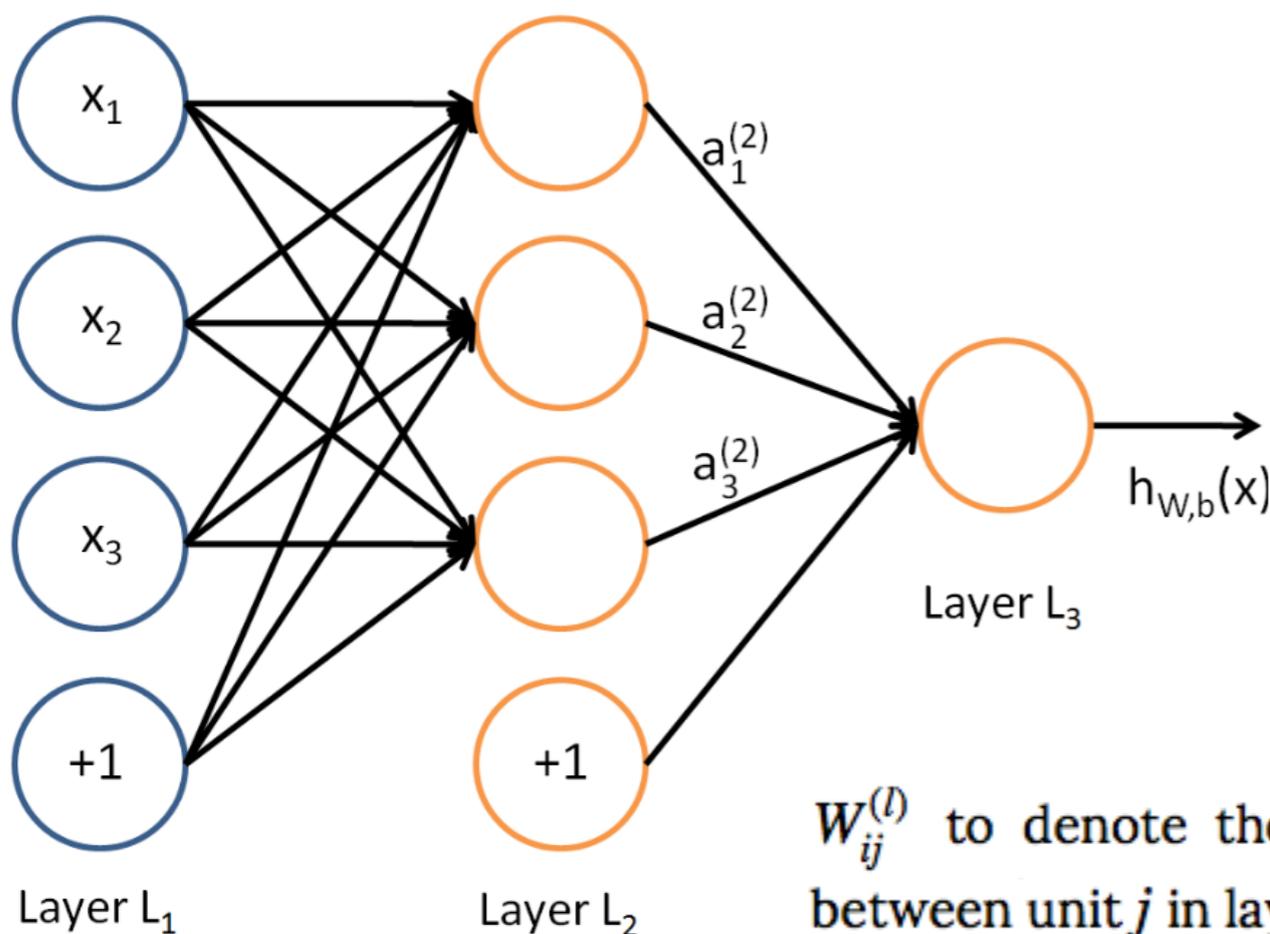
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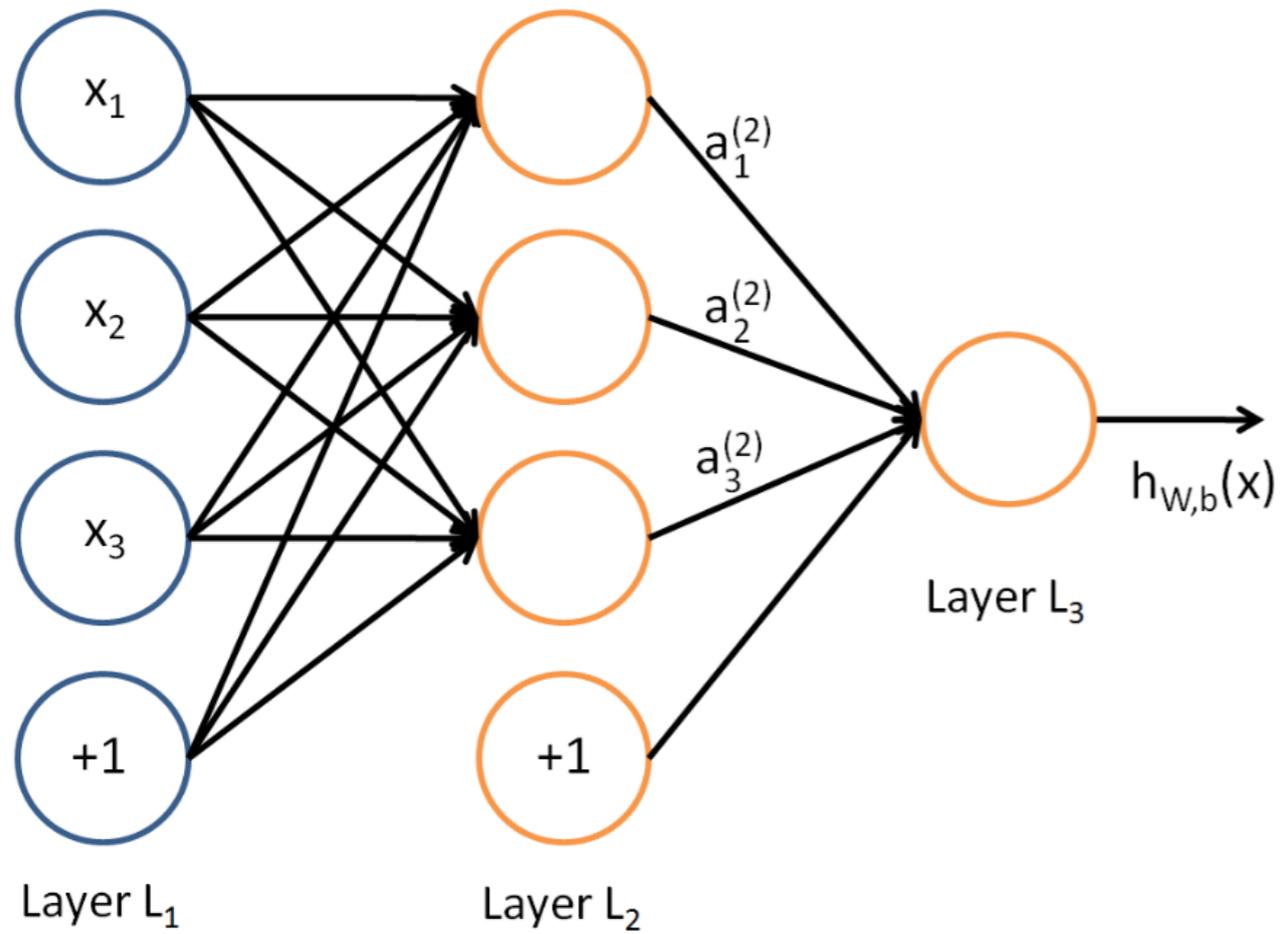
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Our neural network has parameters  $(W, b) = (W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)})$

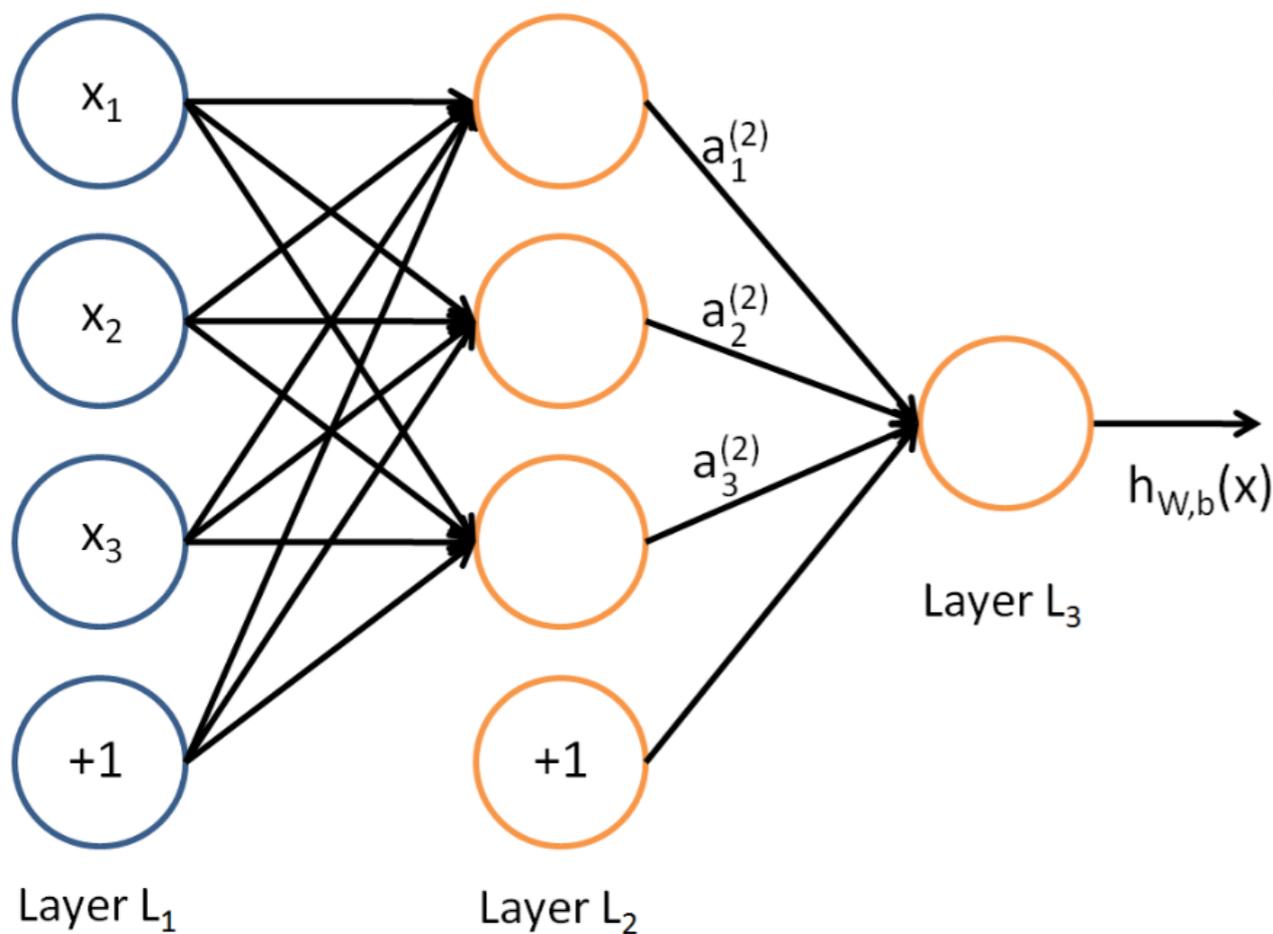
# Artificial Neural Networks

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# Artificial Neural Networks

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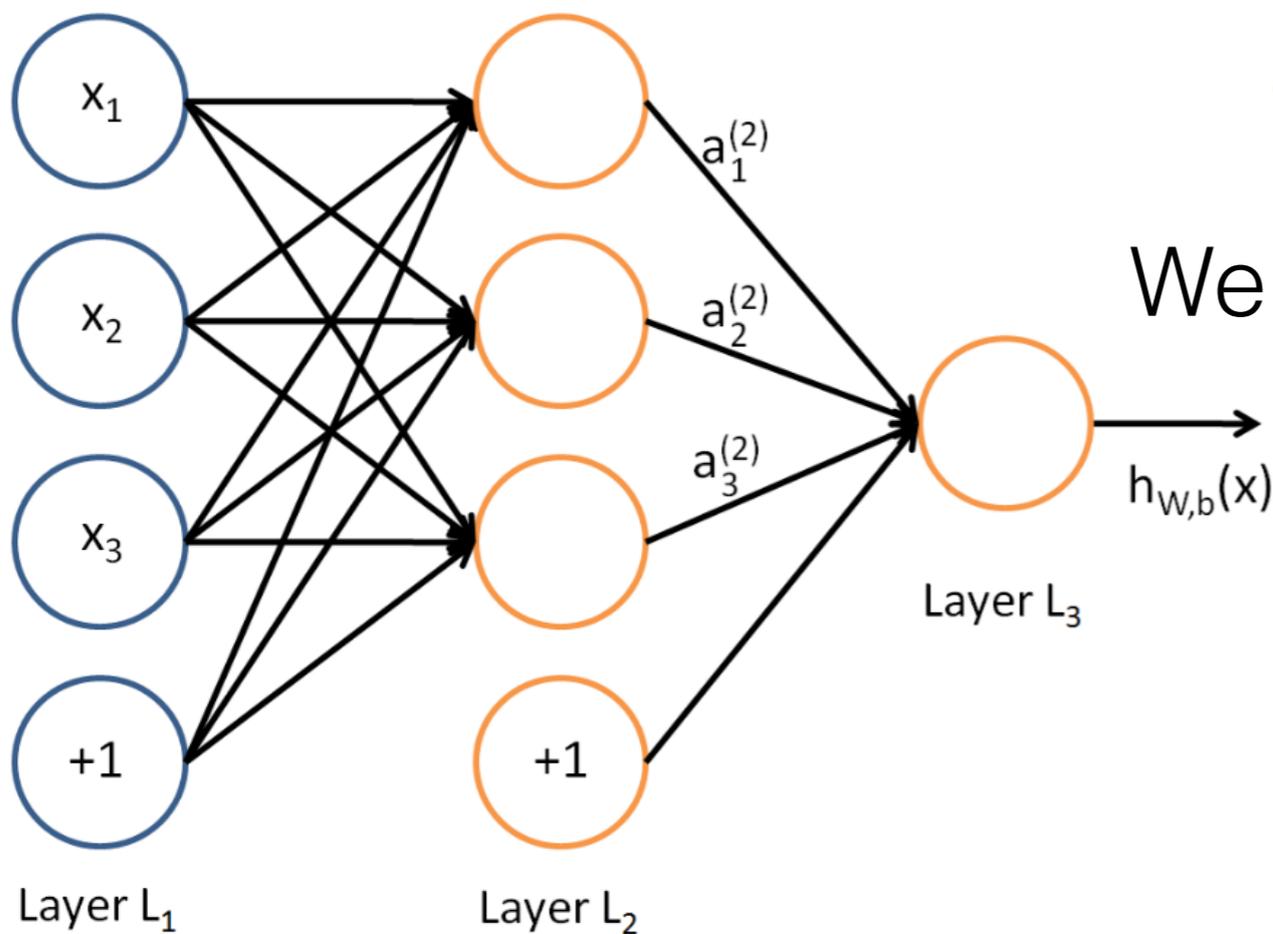
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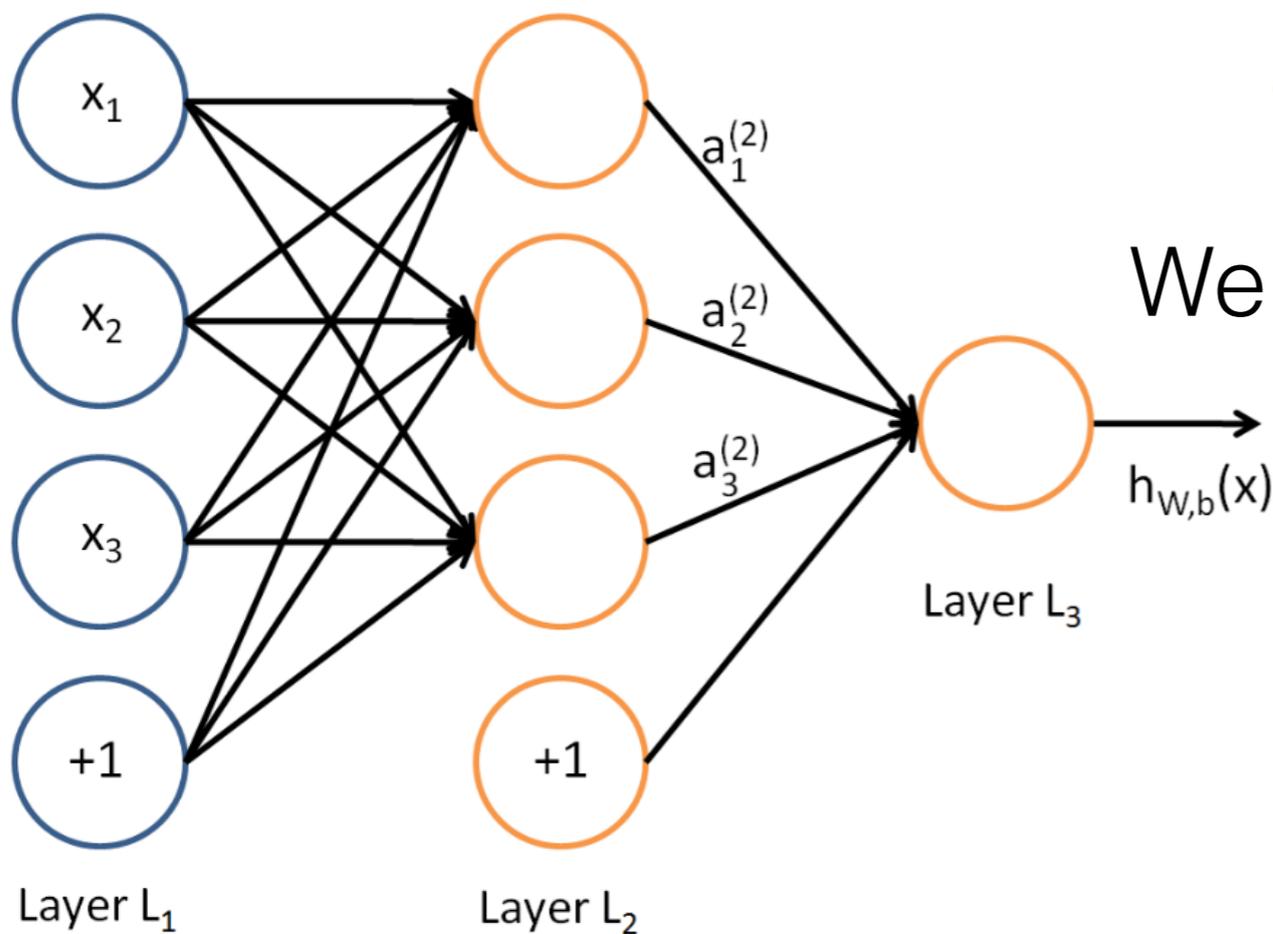
# Artificial Neural Networks



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# Artificial Neural Networks

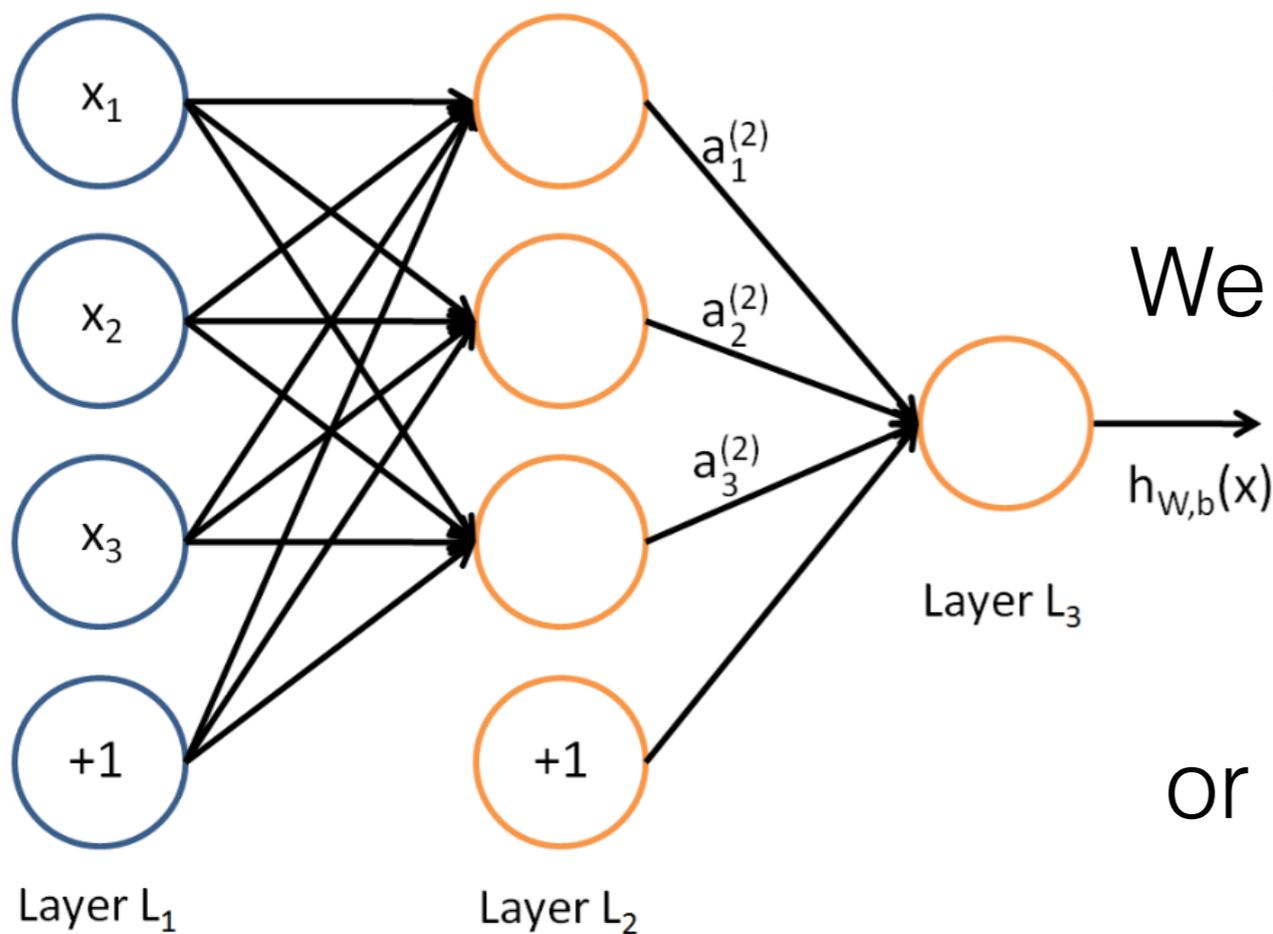


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# Artificial Neural Networks



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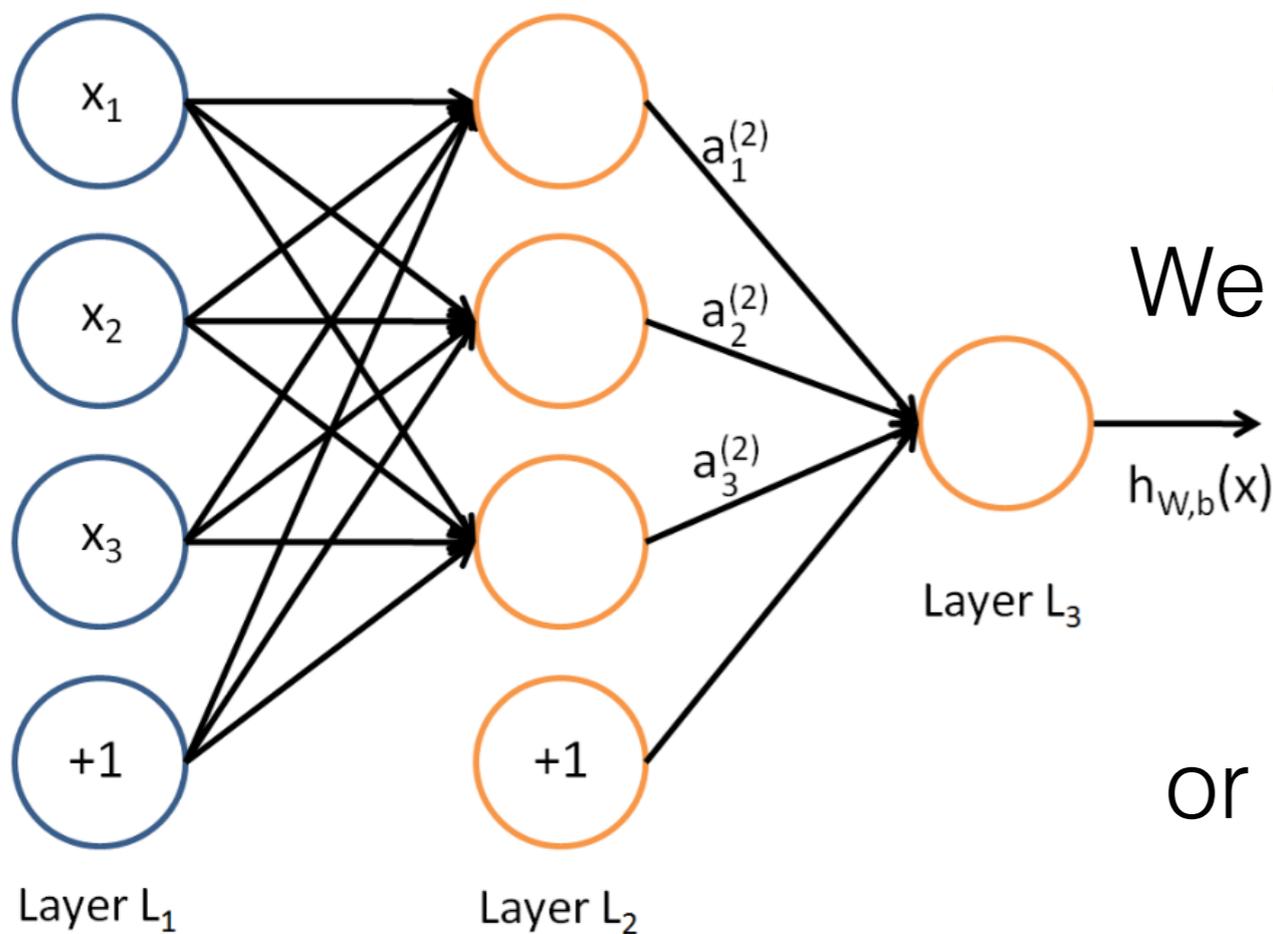
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or more generally as

# Artificial Neural Networks



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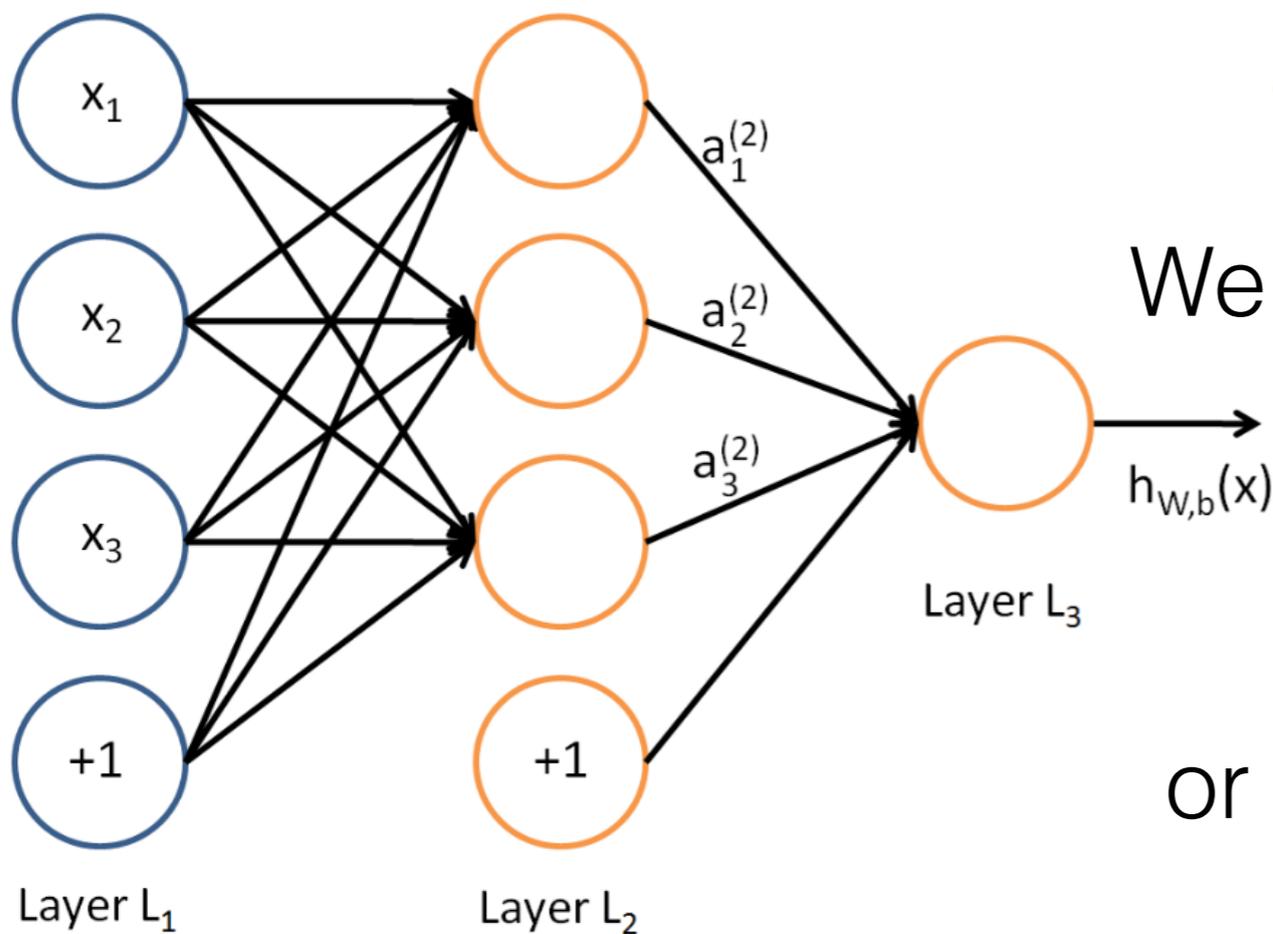
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# Artificial Neural Networks



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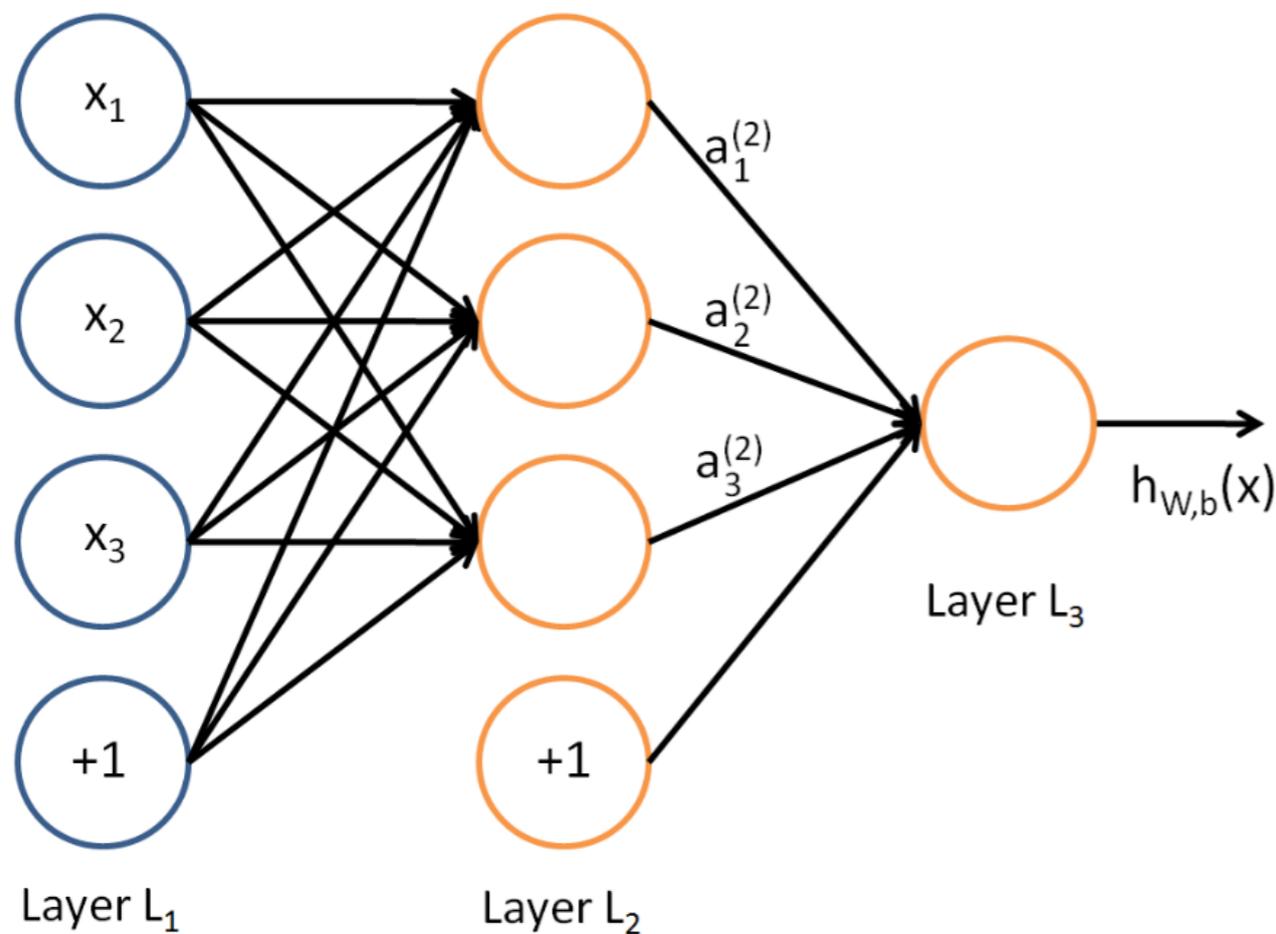
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$$a^{(l+1)} = f(z^{(l+1)})$$

This is a matrix operation.

# Artificial Neural Networks

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**Input:** Set the corresponding activation  $x_1$  for the input layer and initialize weights.

**Feedforward:** For each  $l=2,3, \dots, L$  compute

$$z^{(l+1)} = W^{(l)} a^{(l)} + b^{(l)}$$
$$a^{(l+1)} = f(z^{(l+1)})$$

**Output:** compute cost function.

$$J(W, b; x, y) = \frac{1}{2} \|h_{W,b}(x) - y\|^2$$

**Gradient:** compute gradient.

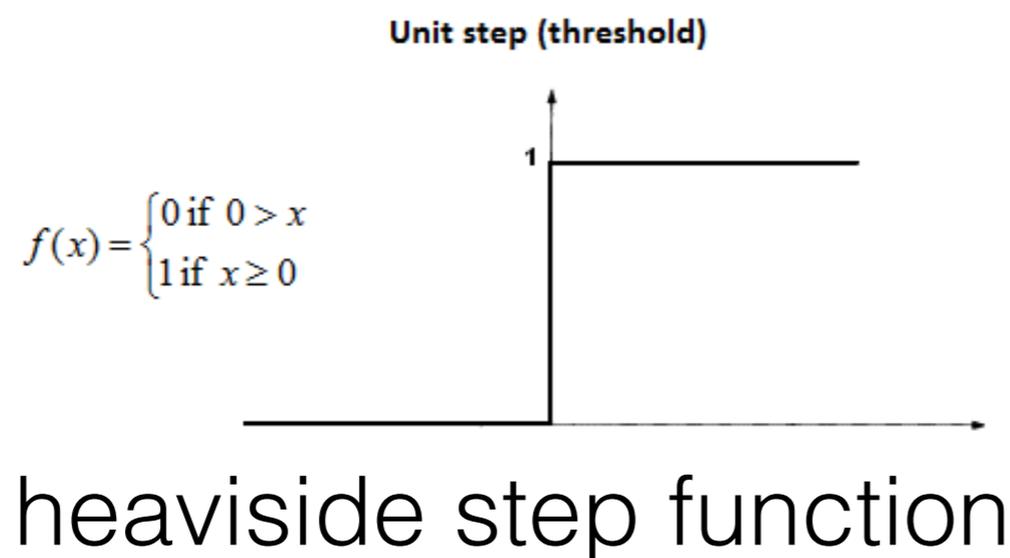
**Backpropagate:** update the weights. Go to feedforward.

# Artificial Neural Networks

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## Activation Function

- translates the input signals to output signals.
- inspired by biological activation that turns information transfer on/off from one neuron to next.
- the simplest form is binary, meaning either the neuron is firing or not.

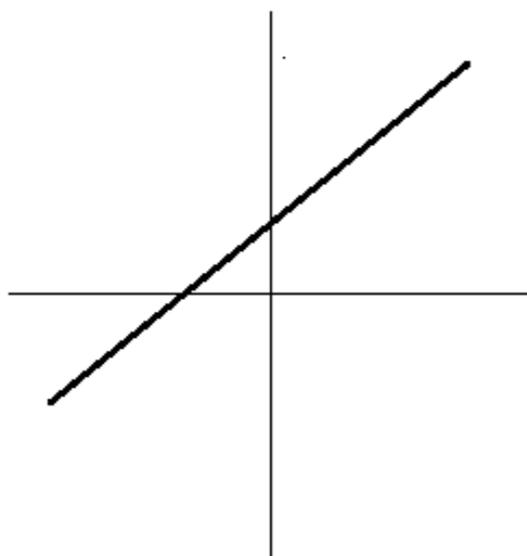


- obviously, this function transfers only binary information.

# Artificial Neural Networks

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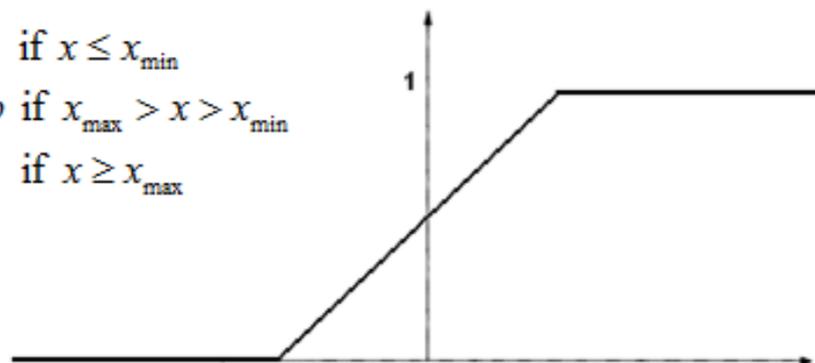
Linear



- a linear activation function transforms the weighted sum inputs of the neuron to an output using a linear response.
- this model has unstable convergence because neuron inputs along favoured paths tend to increase without bound, as this function is not normalizable.

Piecewise Linear

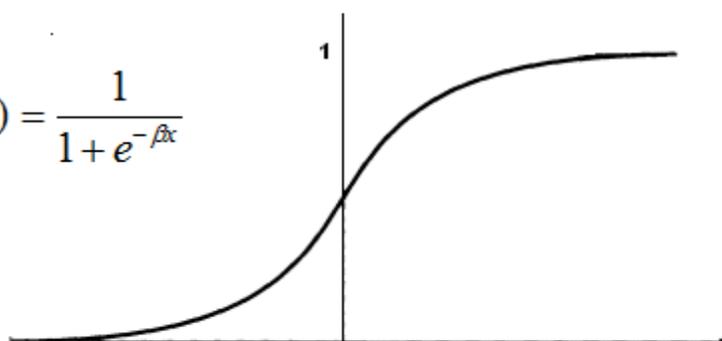
$$f(x) = \begin{cases} 0 & \text{if } x \leq x_{\min} \\ mx + b & \text{if } x_{\max} > x > x_{\min} \\ 1 & \text{if } x \geq x_{\max} \end{cases}$$



- overcomes the drawback of linear.
- the function is normalizable.

Sigmoid

$$f(x) = \frac{1}{1 + e^{-\beta x}}$$



- overcomes the drawback of piecewise linear.
- smooth transition
- better resamples biological response
- popular choice

# Artificial Neural Networks

## Gradient-Descent Procedure

A method that modifies the weights to reduce the cost function:

$$J(W, b; x, y) = \frac{1}{2} \|h_{W,b}(x) - y\|^2$$

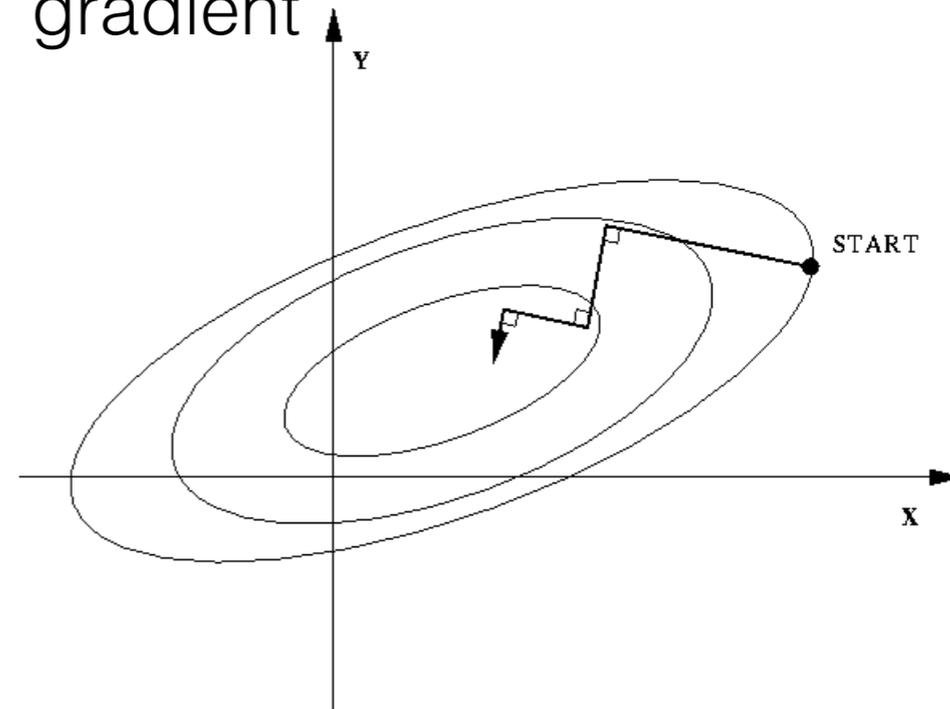
**Algorithm:**

$$w_{ij}[n + 1] = w_{ij}[n] + \overset{\text{step size}}{\eta} g(w_{ij}[n])$$

improved weight

current weight

gradient



# Artificial Neural Networks

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## Deep Neural Networks

If we add more hidden layers we are doing deep learning

Pros: It can model more complex patterns of the data

Cons: It is prone to overfitting and increased computing time

