## Fundamentals of Deep (Artificial) Neural Networks (DNN)

Gregory Tsagkatakis

CSD – UOC & ICS – FORTH

http://users.ics.forth.gr/~greg/

### The Big Data era





### The Big Data era in Astronomy

Sky Survey Project	Volume	Velocity	Variety
Sloan Digital Sky Survey (SDSS)	50 TB	200 GB per day	Images, redshifts
Large Synoptic Survey Telescope (LSST )	~ 200 PB	30 TB per day	lmages, catalogs
Square Kilometer Array (SKA)	~ 4.6 EB	150 TB per day	lmages, redshifts

Garofalo, Mauro, Alessio Botta, and Giorgio Ventre. "Astrophysics and Big Data: Challenges, Methods, and Tools." Proceedings of the International Astronomical Union 12.S325 (2016)

#### Accelerated growth



### Brief history of DL



Why Today?

Lots of Data



Why Today?

#### Lots of Data

#### **Deeper Learning**



Why Today?

Lots of Data

**Deep Learning** 

More Power





https://blogs.nvidia.com/blog/2016/01/12/acceleratingai-artificial-intelligence-gpus/ https://www.slothparadise.com/what-is-cloudcomputing/

### Apps: Gaming



#### Machine learning is everywhere



### Deep Learning

#### Inspiration from brain

- 86Billion neurons
- > 10<sup>14</sup>-10<sup>15</sup> synapses



Brain neurons (billions) Elephant 251 Marmoset 0.634 Rhesus monkey 33 Gorilla ar. 22 Chimpanzee 86 Human Sources: Suzana Herculano-Houzel; Marino, L. Brain Behav Evol 1998;51;230-238 Cerebral cortex neurons (billions) 5.6 AN Elephant 3 Marmoset 0.245 Rhesus monkey 1.7 Gorilla 9.1 1 6 Chimpanzee 16.3 Human Sources: Suzana Herculano-Houzel; Marino, L. Brain Behav Evol 1998;51:230-238

#### Key components of ANN

> Architecture (input/hidden/output layers)



### Key components of ANN

> Architecture (input/hidden/output layers)



### Key components of ANN

- > Architecture (input/hidden/output layers)
- > Weights
- Activations



#### Perceptron: an early attempt

Activation function  

$$\hat{f}(x) = \sigma(w \cdot x + b) \quad \sigma(y) = \begin{cases} 1, & y > 0 \\ 0, & o/w \end{cases}$$

Need to tune w and b



#### Multilayer perceptron



A mostly complete chart of



### Training & Testing

Training: determine weights

- Supervised: labeled training examples
- Unsupervised: no labels available
- Reinforcement: examples associated with rewards

Testing (Inference): apply weights to new examples



### Training DNN

- **1**. Get batch of data
- 2. Forward through the network -> estimate loss
- 3. Backpropagate error
- 4. Update weights based on gradient



### Backpropagation

<u>Chain Rule in Gradient Descent:</u> Invented in 1969 by Bryson and Ho

**Defining a loss/cost function** 

$$J(x, y; \theta) = \frac{1}{2} \sum (y - f(x; \theta))^2$$

Assume a function

$$f(x;\theta) = w^T x + b \quad , \quad \theta = \{w,b\}$$

and associated predictions  $\hat{y} = f(x; \theta)$ 

Examples of Loss function

•Hinge  $J(\hat{y}, y) = max\{0, 1 - \hat{y}y\}$ •Exponential  $J(\hat{y}, y) = exp(-\hat{y}y)$ •Logistic  $J(\hat{y}, y) = log_2(1 + exp(-\hat{y}y))$ 



#### Gradient Descent



#### Backpropagation

Given:  $\boldsymbol{y} = g(\boldsymbol{u})$  and  $\boldsymbol{u} = h(\boldsymbol{x})$ . Chain Rule:  $\frac{dy_i}{dx_k} = \sum_{j=1}^J \frac{dy_i}{du_j} \frac{du_j}{dx_k}, \quad \forall i, k$ 



#### Backpropagation



**Chain rule:** 

• Single variable

• Multiple variables

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}.$$
$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j}\frac{\partial y_j}{\partial x_i}.$$

https://google-developers.appspot.com/machinelearning/crash-course/backprop-scroll/

### Optimization algorithms

Optimization algorithm	Core idea	Pros	Cons
SGD [140]	Computes the gradient of mini-batches iteratively and updates the parameters	• Easy to implement	<ul> <li>Setting a global learning rate required</li> <li>Algorithm may get stuck on saddle points or local minima</li> <li>Slow in terms of convergence</li> <li>Unstable</li> </ul>
Nesterov's momentum [125]	Introduces momentum to maintain the last gradient direction for the next update	<ul> <li>Stable</li> <li>Faster learning</li> <li>Can escape local minima</li> </ul>	• Setting a learning rate needed
Adagrad [126]	Applies different learning rates to different parameters	<ul> <li>Learning rate tailored to each parameter</li> <li>Handle sparse gradients well</li> </ul>	<ul> <li>Still requires setting a global learning rate</li> <li>Gradients sensitive to the regularizer</li> <li>Learning rate becomes very slow in the late stages</li> </ul>
Adadelta [141]	Improves Adagrad, by applying a self-adaptive learning rate	<ul> <li>Does not rely on a global learning rate</li> <li>Faster speed of convergence</li> <li>Fewer hyper-parameters to adjust</li> </ul>	• May get stuck in a local minima at late training
RMSprop [140]	Employs root mean square as a constraint of the learning rate	<ul> <li>Learning rate tailored to each parameter</li> <li>Learning rate do not decrease dramatically at late training</li> <li>Works well in RNN training</li> </ul>	<ul> <li>Still requires a global learning rate</li> <li>Not good at handling sparse gradients</li> </ul>
Adam [127]	Employs a momentum mechanism to store an exponentially decaying average of past gradients	<ul> <li>Learning rate stailored to each parameter</li> <li>Good at handling sparse gradients and non-stationary problems</li> <li>Memory-efficient</li> <li>Fast convergence</li> </ul>	• It may turn unstable during training

#### Visualization



#### **Training Characteristics**



# Supervised Learning

### Supervised Learning

Data Model Labels Prediction

**Exploiting prior knowledge** 

- Expert users
- Crowdsourcing
- Other instruments



#### **Support Vector Machines**

Binary classification



#### **Support Vector Machines**

- Binary classification
- Kernels <-> non-linearities



#### **Support Vector Machines**

- Binary classification
- Kernels <-> non-linearities

#### **Random Forests**

Multi-class classification





#### **Support Vector Machines**

- Binary classification
- Kernels <-> non-linearities

#### **Random Forests**

- Multi-class classification
- Markov Chains/Fields
  - Temporal data

#### State-of-the-art (since 2015)

Deep Learning (DL)

Convolutional Neural Networks (CNN) <-> Images

Recurrent Neural Networks (RNN) <-> Audio

#### **Convolutional Neural Networks**



(Convolution + Subsampling) + () ... + Fully Connected

#### Convolution operator





Image



Convolved Feature
## **Convolutional Layers**



# **Convolutional Layers**

#### Characteristics

- Hierarchical features
- Location invariance

Parameters

- Number of filters (32,64...)
- Filter size (3x3, 5x5)
- Stride (1)
- Padding (2,4)



"Machine Learning and AI for Brain Simulations" – Andrew Ng Talk, UCLA, 2012

## Activation Layer

#### Introduction of non-linearity

Brain: thresholding -> spike trains



Tanh (Hypertangent)





Gaussian



 $\mathit{gaussian}(x) = e^{-x^2/\sigma^2}$ 

# Activation Layer

#### ReLU: x=max(0,x)

- Simplifies backprop
- Makes learning faster
- Avoids saturation issues
  - ~ non-negativity constraint

#### (Note: The brain)





# Subsampling (pooling) Layers



<-> downsampling

Scale invariance

Parameters

Type

- Filter Size
- Stride

# **Fully Connected Layers**

Full connections to all activations in previous layer

Typically at the end

Can be replaced by conv



# LeNet [1998]





# AlexNet [2012]



Alex Krizhevsky, Ilya Sutskever and Geoff Hinton, <u>ImageNet ILSVRC challenge</u> in 2012 http://vision03.csail.mit.edu/cnn\_art/data/single\_layer.png

## VGGnet [2014]



K. Simonyan, A. Zisserman Very Deep Convolutional Networks for Large-Scale Image Recognition, arXiv technical report, 2014

## VGGnet

		ConvNet C	onfiguration		
A	A-LRN	B	C	D	E
11 weight	11 weight	13 weight	16 weight	16 weight	19 weight
layers	layers	layers	layers	layers	layers
	i	e)			
conv3-64	conv3-64	conv3-64	conv3-64	conv3-64	conv3-64
	LRN	conv3-64	conv3-64	conv3-64	conv3-64
conv3-128	conv3-128	conv3-128	conv3-128	conv3-128	conv3-128
		conv3-128	conv3-128	conv3-128	conv3-128
00000000		10			
conv3-256	conv3-256	conv3-256	conv3-256	conv3-256	conv3-256
conv3-256	conv3-256	conv3-256	conv3-256	conv3-256	conv3-256
			conv1-256	conv3-256	conv3-256
					conv3-256
conv3-512	conv3-512	conv3-512	conv3-512	conv3-512	conv3-512
conv3-512	conv3-512	conv3-512	conv3-512	conv3-512	conv3-512
			conv1-512	conv3-512	conv3-512
					conv3-512
		rpool			
conv3-512	conv3-512	conv3-512	conv3-512	conv3-512	conv3-512
conv3-512	conv3-512	conv3-512	conv3-512	conv3-512	conv3-512
			conv1-512	conv3-512	conv3-512
					conv3-512
		soft	-max		

D: VGG16 E: VGG19 All filters are 3x3

More layers smaller filters

# Inception (GoogLeNet, 2014)



Inception module with dimensionality reduction

#### Residuals



## ResNet, 2015



He, Kaiming, et al. "Deep residual learning for image recognition." IEEE CVPR. 2016.

## Dropout



Srivastava, Nitish, et al. "Dropout: a simple way to prevent neural networks from overfitting." *Journal of machine learning research*15.1 (2014): 1929-1958.

## **Batch Normalization**

**Input:** Values of x over a mini-batch:  $\mathcal{B} = \{x_{1...m}\}$ ; Parameters to be learned:  $\gamma, \beta$  **Output:**  $\{y_i = BN_{\gamma,\beta}(x_i)\}$   $\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i$  // mini-batch mean  $\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2$  // mini-batch variance  $\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$  // normalize  $y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv BN_{\gamma,\beta}(x_i)$  // scale and shift



Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift [NTRODUCTION Szegedy 2015]

# Transfer Learning



# Transfer Learning



# Layer Transfer - Image



# Deep Learning Applications in Astronomy

Gregory Tsagkatakis

CSD – UOC & ICS – FORTH

http://users.ics.forth.gr/~greg/

# DL for galaxy morphology

Recovery of galaxy parameters for HST images

Simulation of 31K galaxies (24K training), H band PSF, CANDELS survey noise



Tuccillo, D., Etienne Decencière, and Santiago Velasco-Forero. "Deep learning for studies of galaxy morphology." *Proceedings of the International Astronomical Union* 12.S325 (2016): 191-196.

#### DL for of galaxy morphology (con't)



# CNN: Star-galaxy Classification

type	filters	filter size	padding	non-linearity	initial weights	initial biases
convolutional	32	5×5	-	leaky ReLU	orthogonal	0.1
convolutional	32	3×3	1	leaky ReLU	orthogonal	0.1
pooling	-	$2 \times 2$	-	-	-	-
convolutional	64	$3 \times 3$	1	leaky ReLU	orthogonal	0.1
convolutional	64	$3 \times 3$	1	leaky ReLU	orthogonal	0.1
convolutional	64	$3 \times 3$	1	leaky ReLU	orthogonal	0.1
pooling	-	$2 \times 2$	-	-	-	-
convolutional	128	$3 \times 3$	1	leaky ReLU	orthogonal	0.1
convolutional	128	$3 \times 3$	1	leaky ReLU	orthogonal	0.1
convolutional	128	$3 \times 3$	1	leaky ReLU	orthogonal	0.1
pooling	-	$2 \times 2$	-	-	-	-
fully-connected	2048	-	-	leaky ReLU	orthogonal	0.01
fully-connected	2048	-	-	leaky ReLU	orthogonal	0.01
fully-connected	2	-	-	softmax	orthogonal	0.01

Kim, Edward J., and Robert J. Brunner. "Star-galaxy classification using deep convolutional neural networks." *Monthly Notices of the Royal Astronomical Society* (2016): stw2672.

Star



(a) Input (5 bands×44×44)



(b) Layer 1 (32 maps×40×40)



(c) Layer 3 (64 maps×20×20)



(d) Layer 6 (128 maps×10×10)



(a) Input (5 bands×44×44)

(b) Layer 1 (32 maps×40×40)

(c) Layer 3 (64 maps×20×20)



(d) Layer 6 (128 maps×10×10)

# Gravitational Lensing





# CNN for lensing

#### CNNs in Kilo Degree Survey

21789 colour-magnitude selected Luminous Red Galaxies, of which 3 are known lenses, the CNN retrieves 761 strong-lens candidates and correctly classifies 2/3 of known lenses.



Petrillo, C. E., C. Tortora, S. Chatterjee, G. Vernardos, et al. "Finding strong gravitational lenses in the Kilo Degree Survey with convolutional neural networks." Monthly Notices of the Royal Astronomical Society 472, no. 1 (2017)

# DeepLens

#### Training

20,000 LSST-like observations

#### Testing

for a rejection rate of non-lenses of 99%, a completeness of 90% can be achieved for lenses with Einstein radii larger than 1.400 and S/N larger than 20 on individual g-band LSST exposures.



Lanusse, Francois, et al. "CMU DeepLens: Deep Learning For Automatic Image-based Galaxy-Galaxy Strong Lens Finding." arXiv preprint arXiv:1703.02642 (2017).

# Detecting strong lensing

- Strong galaxy-galaxy lensing systems
- CA-FR-HA Telescope Legacy Survey (CFHTLS)
- Ensemble of trained DL networks
- Search of 1.4 million early type galaxies selected from the survey catalog as potential deflectors,
- Identified 2,465 candidates (117 previously known lens candidates, 29 confirmed lenses, 266 novel probable or potential lenses and 2097 false positives.

Jacobs, Colin, et al. "Finding strong lenses in CFHTLS using convolutional neural networks." Monthly Notices of the Royal Astronomical Society 471.1 (2017)

#### Fast Strong Gravitational Lenses analysis

- ➤ Typical ML approaches: single lens → few weeks & experts
- Estimation of lensing parameters via CNN
  - Singular Isothermal Ellipsoid density profile
  - Parameters: Einstein radius, complex ellipticity, the coordinates of the lens center
- Lens removal through ICA



Hezaveh, Yashar D., Laurence Perreault Levasseur, and Philip J. Marshall. "Fast automated analysis of strong gravitational lenses with convolutional neural networks." *Nature* 548.7669 (2017)

# **Exoplanet detection**



Pearson, Kyle A., Leon Palafox, and Caitlin A. Griffith. "Searching for exoplanets using artificial intelligence." Monthly Notices of the Royal Astronomical Society 474.1 (2017): 478-491.

## Exoplanet detection



## **Exoplanet** detection



Pearson, Kyle A., Leon Palafox, and Caitlin A. Griffith. "Searching for exoplanets using artificial intelligence." Monthly Notices of the Royal Astronomical Society 474.1 (2017): 478-491.

## Quasar micro-lensing light curves

Use CNN to model quasar microlensing light curves and extract the size and temperature profile of the accretion disc.



G. Vernardos and G. Tsagkatakis "Quasar microlensing light curve analysis using deep machine learning", Monthly Notices of the Royal Astronomical Society, Vol. 486 (2), pp. 1944–1952, June 2019,

# Other applications

- Classifying Radio Galaxies With Convolutional Neural Network<sup>1</sup>
- Deep-HITS: Rotation Invariant Convolutional Neural Network For Transient Detection<sup>2</sup>
- Galaxy surface brightness profile<sup>3</sup>

Gravitational wave detection<sup>4</sup>

- 1. Aniyan AK, Thorat K. Classifying Radio Galaxies with the Convolutional Neural Network. The Astrophysical Journal Supplement Series. 2017 Jun 13
- 2. Cabrera-Vives G, Reyes I, Förster F, Estévez PA, Maureira JC. Deep-HiTS: Rotation invariant convolutional neural network for transient detection. The Astrophysical Journal. 2017 Feb 10
- Tuccillo D, Huertas-Company M, Decencière E, Velasco-Forero S, Domínguez Sánchez H, Dimauro P. Deep learning for galaxy surface brightness profile fitting. Monthly Notices of the Royal Astronomical Society. 2017 Dec 11
- 4. George, Daniel, and E. A. Huerta. "Deep Learning for real-time gravitational wave detection and parameter estimation: Results with Advanced LIGO data." *Physics Letters B* 778 (2018): 64-70.

# GANs for deconvolution

#### 4,550 SDSS images of nearby galaxies at 0:01 < z < 0:02



Schawinski, Kevin, et al. "Generative Adversarial Networks recover features in astrophysical images of galaxies beyond the deconvolution limit." *arXiv preprint arXiv:1702.00403* (2017).

## TensorFlow

Deep learning library, open-sourced by Google (11/2015)

TensorFlow provides primitives for

- defining functions on tensors
- automatically computing their derivatives

What is a tensor

What is a computational graph

Material from lecture by Bharath Ramsundar, March 2018, Stanford



# Introduction to Keras

#### Official high-level API of TensorFlow

- Python
- 250K developers
- Developed by Francois Chollet

#### Same front-end <-> Different back-ends

- TensorFlow (Google)
- CNTK (Microsoft)
- MXNet (Apache)
- Theano (RIP)

#### Hardware

- GPU (Nvidia)
- CPU (Intel/AMD)
- TPU (Google)

Companies: AWS, Uber, Google, Nvidia...



# Keras API TensorFlow / CNTK / MXNet / Theano / ... GPU CPU TPU
## Keras models

Installation

Anaconda -> Tensorflow -> Keras

Build-in

- Conv1D, Conv2D, Conv3D...
- MaxPooling1D, MaxPooling2D, MaxPooling3D...
- Dense, Activation, RNN...

#### The Sequential Model

- Very simple
- Single-input, Single-output, sequential layer stacks

#### The functional API

- Mix & Match
- Multi-input, multi-output, arbitrary static graph topologies

## Sequential API

- >> import keras
- >> from keras import layers
- >> model = Sequential()
- >> model.add(layers.Dense(24, activation='relu', input\_shape(10,)))
- >> model.add(layers.Dense(20, activation='relu'))
- >> model.add(layers.Dense(10, activation='softmax'))
- >> model.fit(x\_train, y\_train, epochs=5, batch\_size=32)

## Functional API

>> import keras

- >> from keras import layers
- >> inputs = keras.Input(shape=(10,))
- >> x = layers.Dense(20, activation='relu')(inputs)
- >> x = layers.Dense(20, activation='relu')(x)
- >> outputs = layers.Dense(10, activation='softmax')(x)
- >> model = keras.Model(inputs, outputs)
- >> model.fit(x\_train, y\_train, epochs=5, batch\_size=32)

## Sequential

>>from keras.models import Sequential

>>model = Sequential()

>> from keras.layers import Dense

>> model.add(Dense(units=64, activation='relu', input\_dim=100))

>> model.add(Dense(units=10, activation='softmax'))

>> model.compile(loss='categorical\_crossentropy',
optimizer='sgd', metrics=['accuracy'])

>> model.fit(x\_train, y\_train, epochs=5, batch\_size=32)

>> loss\_and\_metrics = model.evaluate(x\_test, y\_test, batch\_size=128)

>> classes = model.predict(x\_test)

## Functional

- >> from keras.layers import Input, Dense
- >> from keras.models import Model
- >> inputs = Input(shape=(784,))
- >> x = Dense(64, activation='relu')(inputs)
- >> x = Dense(64, activation='relu')(x)
- >> predictions = Dense(10, activation='softmax')(x)
- >> model = Model(inputs=inputs, outputs=predictions)
- >> model.compile(optimizer='SGD',loss='categorical\_crossentropy', metrics=['accuracy'])
- >> model.fit(data, labels)

### Case study #1: Galaxy morphology

### **Euclid mission**

Mission: map the dark universe

Planned launch in 2022





## Case study



# Kaggle kernels

https://www.kaggle.com/greg1982/astroschoolmorphology