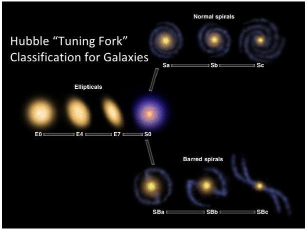
Introduction to supervised learning: from linear models, through Boosting to SVM

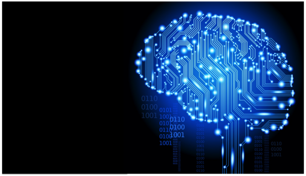
Stéphane Canu
asi.insa-rouen.fr/enseignants/~scanu
scanu@insa-rouen.fr



Workshop on Machine Learning

February 14, 2019

Introduction to supervised learning



Machine learning (AI) for SETI

Leonardo Garrido
@LeonardoGarrido

Suivre

Breakthrough Listen is also applying the successful machine learning algorithm to find new kinds of signals that could be coming from extraterrestrial civilizations ...

Traduire le Tweet

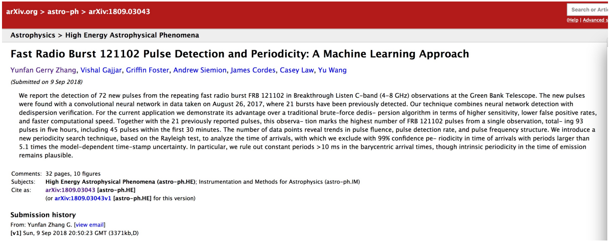
AI helps track down mysterious cosmic radio bursts

Using machine learning techniques, Breakthrough Listen researchers have been able to find many more enigmatic fast radio bursts

news.berkeley.edu

17:55 - 14 sept. 2018

Machine learning (AI) for SETI: the paper



arXiv.org > astro-ph > arXiv:1809.03043

Search or Arti

(Help | Advanced s

Astrophysics > High Energy Astrophysical Phenomena

Fast Radio Burst 121102 Pulse Detection and Periodicity: A Machine Learning Approach

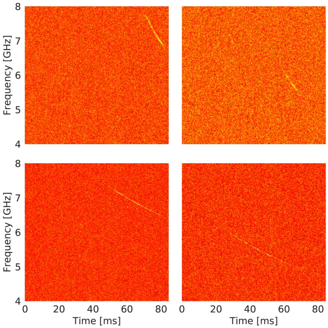
Yunfan Gerry Zhang, Vishal Gajjar, Griffin Foster, Andrew Siemion, James Cordes, Casey Law, Yu Wang

(Submitted on 9 Sep 2018)

We report the detection of 72 new pulses from the repeating fast radio burst FRB 121102 in Breakthrough Listen C-band (4-8 GHz) observations at the Green Bank Telescope. The new pulses were found with a convolutional neural network in data taken on August 26, 2017, where 21 bursts have been previously detected. Our technique combines neural network detection with dedispersion verification. For the current application we demonstrate its advantage over a traditional brute-force dedis- persion algorithm in terms of higher sensitivity, lower false positive rates, and faster computational speed. Together with the 21 previously reported pulses, this observa- tion marks the highest number of FRB 121102 pulses from a single observation, total- ing 93 pulses in five hours, including 45 pulses within the first 30 minutes. The number of data points reveal trends in pulse fluence, pulse detection rate, and pulse frequency structure. We introduce a new periodicity search technique, based on the Rayleigh test, to analyze the time of arrivals, with which we exclude with 99% confidence pe- riodicity in time of arrivals with periods larger than 5.1 times the model-dependent time-stamp uncertainty. In particular, we rule out constant periods >10 ms in the barycentric arrival times, though intrinsic periodicity in the time of emission remains plausible.

Comments: 32 pages, 10 figures
Subjects: **High Energy Astrophysical Phenomena (astro-ph.HE)**; Instrumentation and Methods for Astrophysics (astro-ph.IM)
Cite as: arXiv:1809.03043 [astro-ph.HE]
(or arXiv:1809.03043v1 [astro-ph.HE] for this version)

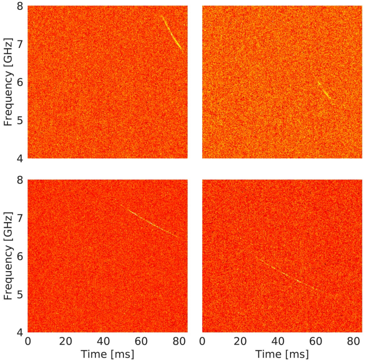
Submission history
From: Yunfan Zhang G. [view email]
[v1] Sun, 9 Sep 2018 20:50:23 GMT (3371kb,D)



- August 26, 2017: 21 bursts have been previously detected.
- Machine learning: 72 new detections

Machine learning (AI) for SETI: the machine learning

- Data
  - 5 hours listen observations
  - 400000 images,
  - half of which contain simulated pulses



- model
  - inputs: images
  - outut: detection (yes/no)
  - convolutional deep network 17 layers
  - 6.2 million trainable parameters

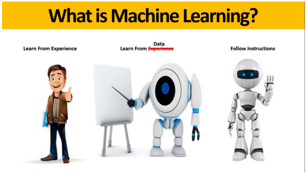
- training
  - training set = 4.5 hours
  - 20 hours on a GPU
  - error converges after 100 epochs to 93%

- combined with dedispersion verification

$$decision = f(image) + noise$$

Plan

1. Introducing example
2. Machine learning
   - Definition attempt
   - Hypothesis set and methods
3. Deep Learning
4. Some practical issues



Machine learning

- model

$$decision = f(image) + noise$$

$$\mathbb{P}(decision, image) \text{ unknown}$$
.

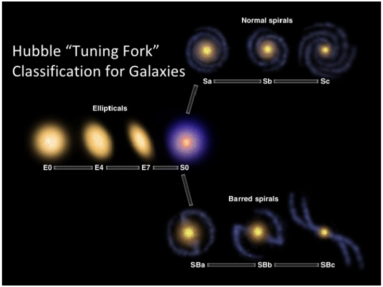
- goal = cost

$$\widehat{f} \text{ estimate } f \text{ from data}$$
.
$$\text{minimize the cost of } \widehat{f}$$
.

- issues: induction

  statistics + unknown distribution + cost + computational issues .

Examples of machine laernig



task	data	performance
predict the type of a galaxy	images	error rate
estimate a frequency	images	quadratic loss
(discover) galaxy type	images	entropy
recommand next line of code	software	reinforcement

https://www.kaggle.com/c/galaxy-zoo-the-galaxy-challenge

Les trois (principales) familles d'apprentissage automatique

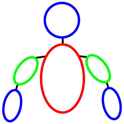
Apprendre à prédire : apprentissage supervisé

Entrée x sorties y

- $y \in \{0, 1\}$ classification binaire ou multiple


- $y \in \mathbf{R}$ régression

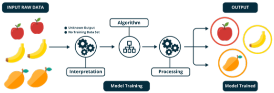

- $y \in \{faible, moyen, fort\}$ ordonnancement
- y structuré

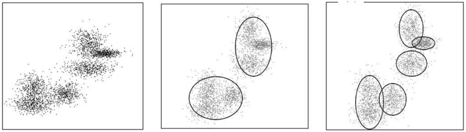



Apprendre à résumer : apprentissage non supervisé

Entrée x seul (pas de y)

- Catégoriser (clustering) : qui se ressemble s'assemble   k-means, CHA

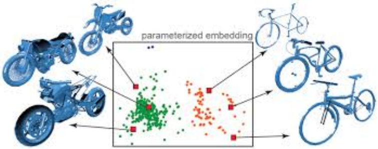




(a) Input data   (b) GMM (K=2)   (c) GMM (K=5)

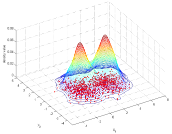
.

- Représenter: $x \in \mathbb{R}^p \longrightarrow z \in \mathbb{R}^d, d \ll p$ ACP, t-SNE, UMAP



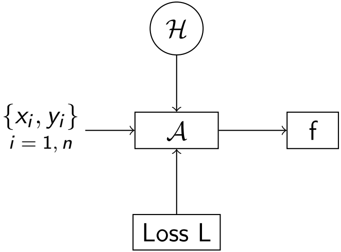
.

- Estimer une densitée $\mathbb{P}(x)$ Parzen,



.

Apprentissage et ensemble d'hypothèses



apprendre c'est :

sélectionner, parmi des hypothèses, la plus cohérente avec les données

Universalité de l'apprentissage

Résultat d'existence

Théorème d'approximation universel

- soit $\varepsilon > 0$ un réel
- quelle que soit la tâche à apprendre $\forall f^{\star}$
- il existe $\hat{f} \in \mathcal{H}$, telle que

$$\|f^{\star} - \hat{f}\| \leq \varepsilon$$

Choisir un ensemble d'hypothèses $\mathcal{H}$ universel

- plus on a d'exemples, plus le modèle doit pouvoir être complexe
- danger : surapprentissage
- question centrale : adapter la complexité du modèle au prolème

Les différents types de modèles universels

- modèles basées sur les variables
  - la notion de dictionnaire (base, polynômes, ondelettes. . .)

$$\hat{f}(x) = \sum_{k=1}^{k} \alpha_k \phi_k(x)$$

- modèles basées sur les exemples
  - plus proches voisins
  - noyaux (SVM)

- combinaison d'éléments simples (partitions)
  - les forêts aléatoires
  - le boosting

- modèles profonds (deep learning)

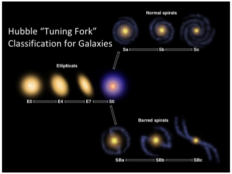
linéaires vs non linéaires

$\rightarrow$ C'est un problème de représentation (extraction de caractéristiques)

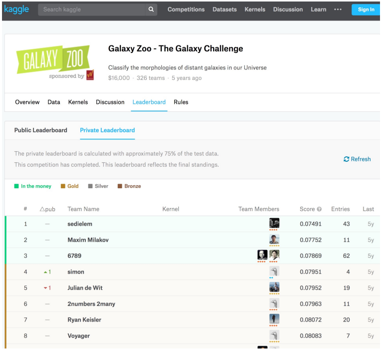
Machine learning for galaxy morphology prediction

Galaxy Zoo - The Galaxy Challenge at Kaggle

- Data
  - training set with 61,578 images
  - test set of 79,975 images
  - Data augmentation



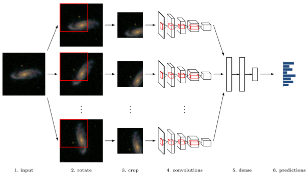
- model
  - inputs: images
  - outut: proba galaxy morphology
  - SVM, GBM,
  - convolutional deep network



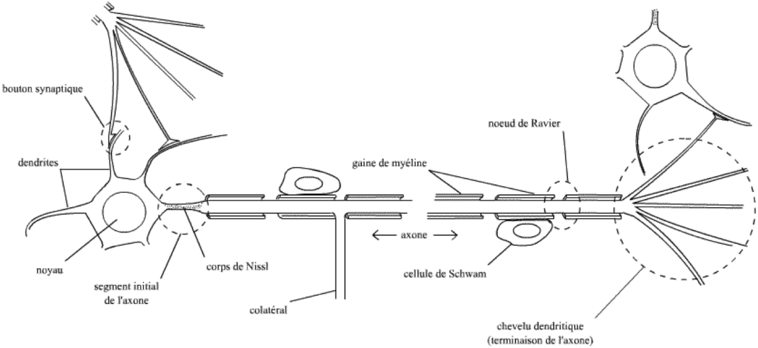
- training accuracy
  - SVM 88%
  - Gradient Boosting 90 %
  - deep learning (CNN) 93%

https://www.kaggle.com/c/galaxy-zoo-the-galaxy-challenge/discussion/7599

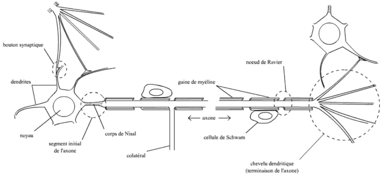
Plan

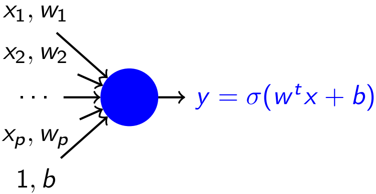


The biological neuron



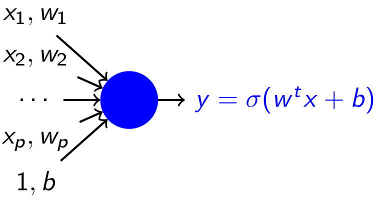
McCulloch & Pitts formal neuron 1943

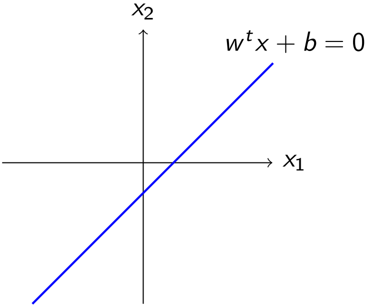




- x input $\in \mathbb{R}^p$
- w weight, b bias
- σ activation function
- y output $\in \mathbb{R}$

The artificial neuron as a linear threshold unit





- x input $\in \mathbb{R}^p$
- w weight, b bias
- a activation, $a = w^t x + b$
- σ activation function
- ϕ transfer function
- y output $\in \mathbb{R}$

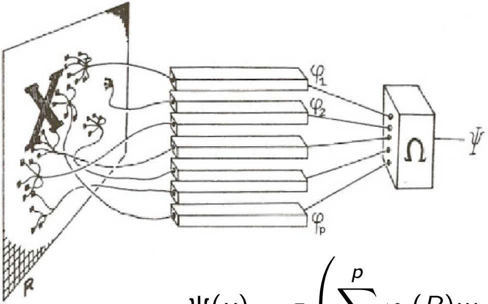
σ activation function (non linear)

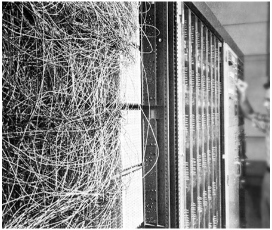
$$\begin{array}{ccc} \mathbb{R} & \mapsto & \mathbb{R} \\ a & \to & y = \sigma(a) \end{array}$$

ϕ transfer function

$$\begin{array}{ccc} \mathbb{R}^p & \mapsto & \mathbb{R} \\ \mathbf{x} & \to & y = \phi(\mathbf{x}) = \sigma(w^t x + b) \end{array}$$

The formal neuron as a learning machine: fit the w





$$\Psi(x) = \sigma\left(\sum_{j=1}^{p} \varphi_j(R) w_j + b\right)$$

Rosenblatt's Perceptron, 1958 (Widrow & Hoff's Adaline, 1960)

given n pairs of input–output data $\mathbf{x}_i = \varphi_j(R_i), t_i, i = 1, n$

find w such that $\underbrace{\sigma(\mathrm{w}^t \mathbf{x}_i)}_{\text{prediction of the model}} = \underbrace{t_i}_{\text{ground truth}}$

Cost minimization (energy-based model)

Minimize a loss	$\displaystyle\min_{\mathrm{w}\in\mathbb{R}^{p+1}} \sum_{i=1}^{n} \mathit{loss}(\mathrm{w})$	$\mathit{loss}(\mathrm{w}) = \big(\sigma(\mathrm{w}^t\mathbf{x}_i) - t_i\big)^2$
Gradient descent	$\mathrm{w} \leftarrow \mathrm{w} - \rho\mathbf{d}$	$\displaystyle\mathbf{d} = \sum_{i=1}^{n} \nabla_{\mathrm{w}}\mathit{loss}(\mathrm{w})$
Stochastic gradient		$\mathbf{d} = \nabla_{\mathrm{w}}\mathit{loss}(\mathrm{w})$

Algorithm 1 Gradient epoch

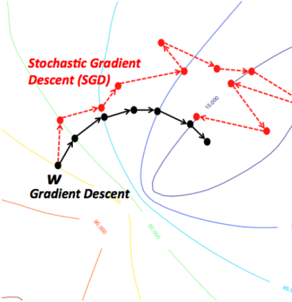
Data: w initialization, ρ stepsize
Result: w
for *i=1,n* **do**
  $\mathbf{x}_i, t_i \leftarrow$ pick a point i
  $\mathbf{d} \leftarrow d + \nabla_{\mathrm{w}}\mathit{loss}(\mathrm{w}, x_i, t_i)$
end
$\mathrm{w} \leftarrow \mathrm{w} - \rho\mathbf{d}$

Algorithm 2 Stochastic gradient

Data: w initialization, ρ stepsize
Result: w
for *i=1,n* **do**
  $\mathbf{x}_i, t_i \leftarrow$ pick a point i
  $\mathbf{d} \leftarrow \nabla_{\mathrm{w}}\mathit{loss}(\mathrm{w}, x_i, t_i)$
  $\mathrm{w} \leftarrow \mathrm{w} - \rho\mathbf{d}$
end

Accelerating the stochastic gradient

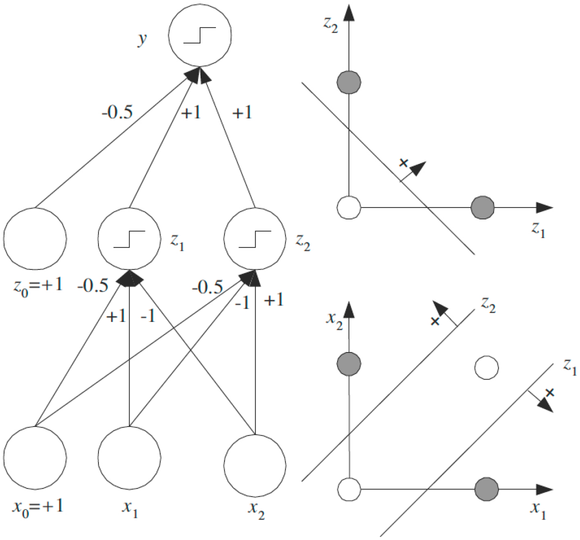
- stochastic average (mini batch)
  - parameters (Polyak and Juditsky, 1992)
  - gradients SAG-A, (Le Roux et al 2012)
  - variance reduction (Johnson, Zhang, 2013)
- convergence acceleration
  - Nesterov's method (1983)
  - momentum (heuristic)
- acceleration and averaging
  - (Dieuleveut, Flammarion & Bach, 2016)
- stepsize adaptation
  - RMSprop (Tieleman & Hinton, 2012)
  - Adaptive Moment Estimation – ADAM (Kingma & Ba, 2015)
  - AMSGRAD (Reddi et al, BPA ICRL 2018)



http://ruder.io/optimizing-gradient-descent/ https://wikidocs.net/3413

Optimization methods for large-scale machine learning L Bottou, FE Curtis, J Nocedal - stat, 2017 -

Non linearity combining linear neurons: the Xor case



Alpaydın, Introduction to Machine Learning, 2010

Neural networks

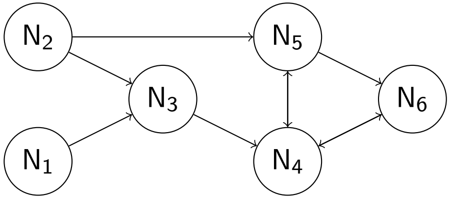
Definition: Neural network

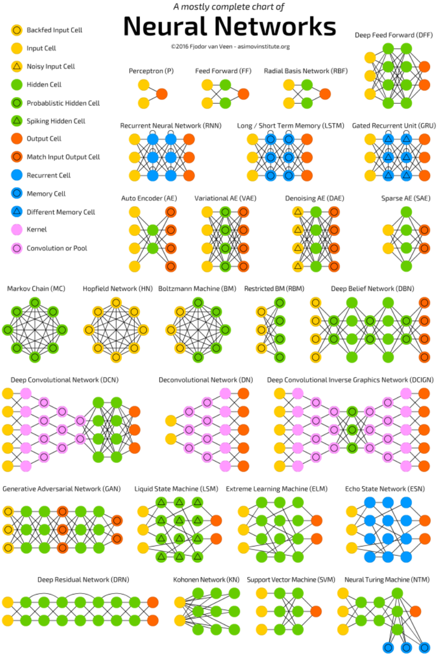
A neural network is an oriented weighted graph of formal neurons

When two neurons are connected (linked by an oriented edge of the graph), the output of the head neuron is used as an input by the tail neuron. It can be seen as a weighted directed graph

3 different neurons are considered:

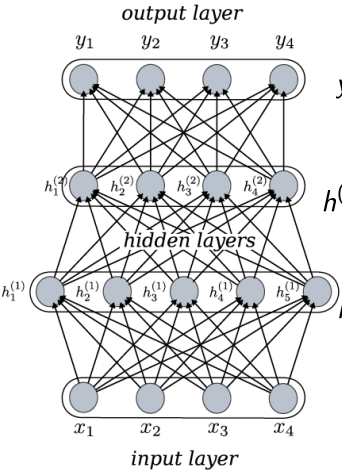
- input neurons (connected with the input)
- output neurons
- hidden neurons





The Asimov Institute: http://www.asimovinstitute.org/neural-network-zoo/

Neural networks propagation and back propagation



$$y = \varphi(W_3 h^{(2)})$$

$$\uparrow$$

$$h^{(2)} = \varphi(W_2 h^{(1)})$$

$$\uparrow$$

$$h^{(1)} = \varphi(W_1 \mathbf{x})$$

$$\uparrow$$

$$\mathbf{x}$$

$$\nabla_{W_3} J = (y - y_a)\varphi'(W_3 h^{(2)})h^{(2)}$$

$$\downarrow$$

$$\nabla_{W_2} J = \nabla_{h^{(2)}} J \varphi'(W_2 h^{(1)})h^{(1)}$$

$$\downarrow$$

$$\nabla_{W_1} J =$$

backpropagation = chain rule (autodiff)

Used to learn internal representation W_1, W_2, W_3

Back propagation is differential learning

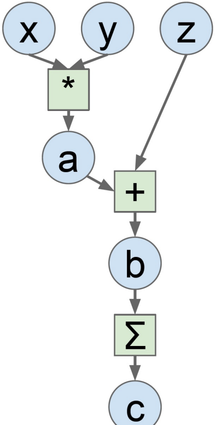
Yann LeCun

5 janvier ·

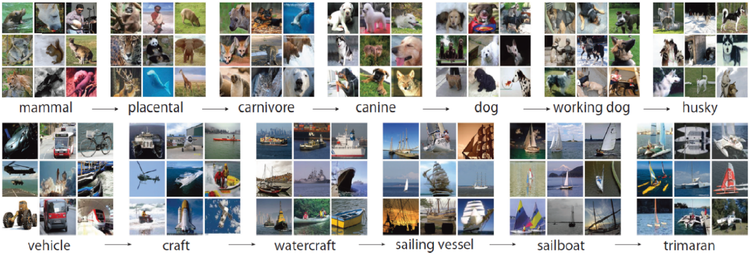
OK, Deep Learning has outlived its usefulness as a buzz-phrase.
Deep Learning est mort. Vive Differentiable Programming!

Numpy

```
import numpy as np
np.random.seed(0)

N, D = 3, 4

x = np.random.randn(N, D)
y = np.random.randn(N, D)
z = np.random.randn(N, D)

a = x * y
b = a + z
c = np.sum(b)

grad_c = 1.0
grad_b = grad_c * np.ones((N, D))
grad_a = grad_b.copy()
grad_z = grad_b.copy()
grad_x = grad_a * y
```



The image net database (Deng et al., 2012)



ImageNet = 15 million high-resolution images of 22,000 categories.
Large-Scale Visual Recognition Challenge (a subset of ImageNet)

- 1000 categories.
- 1.2 million training images,
- 50,000 validation images,
- 150,000 testing images.

www.image-net.org/challenges/LSVRC/2012/

A new fashion in image processing

2012 Teams	%error
Supervision (Toronto)	15.3
ISI (Tokyo)	26.1
VGG (Oxford)	26.9
XRCE/INRIA	27.0
UvA (Amsterdam)	29.6
INRIA/LEAR	33.4

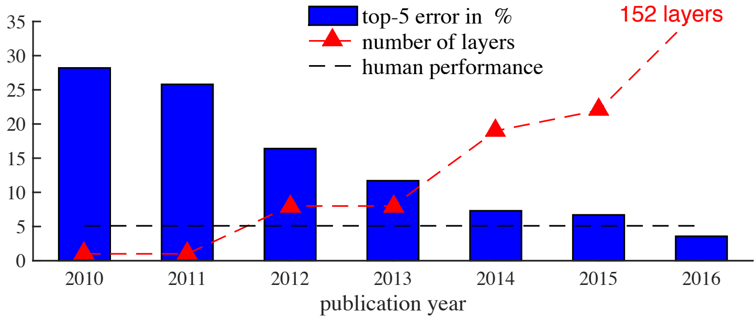
2013 Teams	%error
Clarifai (NYU spinoff)	11.7
NUS (singapore)	12.9
Zeiler-Fergus (NYU)	13.5
A. Howard	13.5
OverFeat (NYU)	14.1
UvA (Amsterdam)	14.2
Adobe	15.2
VGG (Oxford)	15.2
VGG (Oxford)	23.0

2014 Teams	%error
GoogLeNet	6.6
VGG (Oxford)	7.3
MSRA	8.0
A. Howard	8.1
DeeperVision	9.5
NUS-BST	9.7
TTIC-ECP	10.2
XYZ	11.2
UvA	12.1

shallow approaches

deep learning

ImageNet results



2012 Alex Net

2013 ZFNet

2014 VGG

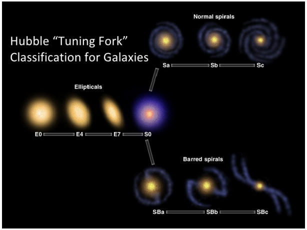
2015 GoogLeNet / Inception

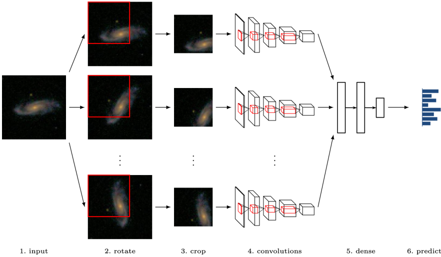
2016 Residual Network

karpathy's blog: `karpathy.github.io/2014/09/02/what-i-learned-from-competing-against-a-convnet-on-imagenet/`

Deep learning for galaxy morphology prediction

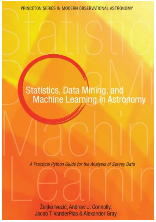
- Data
  - training 61,578 / test 79,975 images
- model
  - inputs: 45 by 45 by 3 arrays of RGB
  - 16 different viewpoints
  - outut: 37 answer probabilities
  - four convolutional layers
  - 42 million trainable parameters
- training
  - Data augmentation, parameter sharing & dropout
  - manual parameter search: more than 100 architectures were evaluated
  - Model averaging
  - 67 hours (accuracy of 98%)



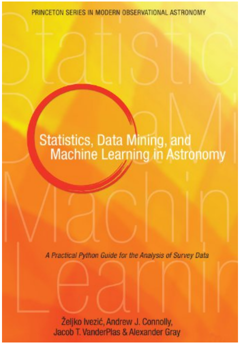


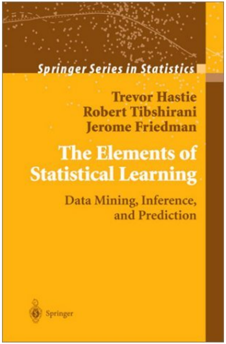
Dieleman, Sander, Kyle W. Willett, and Joni Dambre. "Rotation-invariant convolutional neural networks for galaxy morphology prediction." Monthly notices of the royal astronomical society 450.2 (2015): 1441-1459.

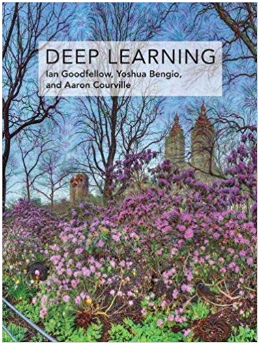
Plan


PRINCETON SERIES IN MODERN OBSERVATIONAL ASTRONOMY
Statistics, Data Mining, and
Machine Learning in Astronomy
A Practical Python Guide for the Analysis of Survey Data
Željko Ivezić, Andrew J. Connolly,
Jacob T. VanderPlas & Alexander Gray

A book to begin with machine learning in astronomy





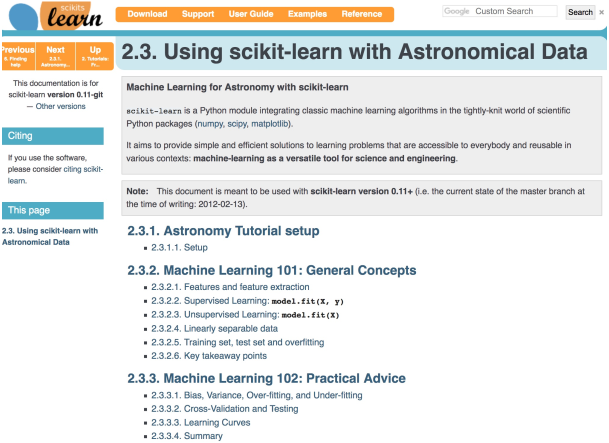


Ivezic, Zeljko, et al. Statistics, **Data Mining, and Machine Learning in Astronomy: A Practical Python Guide for the Analysis of Survey Data**. Princeton University Press, 2014.

`astroml.org`

astroML: code to begin with machine learning in astronomy

Python module for machine learning and data mining built on numpy, scipy, **scikit-learn**, and matplotlib



scikits learn

Download | Support | User Guide | Examples | Reference

Google Custom Search | Search

Previous 6. Finding help | Next 2.3.1. Astronomy... | Up 2., Tutorials: Fr...

This documentation is for scikit-learn **version 0.11-git** — Other versions

Citing

If you use the software, please consider citing scikit-learn.

This page

2.3. Using scikit-learn with Astronomical Data

2.3. Using scikit-learn with Astronomical Data

Machine Learning for Astronomy with scikit-learn

`scikit-learn` is a Python module integrating classic machine learning algorithms in the tightly-knit world of scientific Python packages (numpy, scipy, matplotlib).

It aims to provide simple and efficient solutions to learning problems that are accessible to everybody and reusable in various contexts: **machine-learning as a versatile tool for science and engineering**.

Note: This document is meant to be used with **scikit-learn version 0.11+** (i.e. the current state of the master branch at the time of writing: 2012-02-13).

2.3.1. Astronomy Tutorial setup

- 2.3.1.1. Setup

2.3.2. Machine Learning 101: General Concepts

- 2.3.2.1. Features and feature extraction
- 2.3.2.2. Supervised Learning: `model.fit(X, y)`
- 2.3.2.3. Unsupervised Learning: `model.fit(X)`
- 2.3.2.4. Linearly separable data
- 2.3.2.5. Training set, test set and overfitting
- 2.3.2.6. Key takeaway points

2.3.3. Machine Learning 102: Practical Advice

- 2.3.3.1. Bias, Variance, Over-fitting, and Under-fitting
- 2.3.3.2. Cross-Validation and Testing
- 2.3.3.3. Learning Curves
- 2.3.3.4. Summary

astoML: `github.com/astroML/astroML`

`ogrisel.github.io/scikit-learn.org/sklearn-tutorial/tutorial/astronomy`

AstroNN: code to begin with deep learning in astronomy

Python module for deep learning built on **Keras** (and scikit-learn)

Galaxy10 Tutorial

Introduction

This notebook will demonstrate how to train a simple convolutional neural network with astroNN on Galaxy10 dataset to classify galaxy images.

Galaxy10 is a dataset contains 25753 69x69 pixels colored galaxy images (g, r and i band) separated in 10 classes. Galaxy10 images come from Sloan Digital Sky Survey and labels come from Galaxy Zoo.

There is no guarantee on the accuracy of the labels. Moreover, Galaxy10 is not a balanced dataset and it should only be used for educational or experimental purpose. If you use Galaxy10 for research purpose, please cite Galaxy Zoo and Sloan Digital Sky Survey.

For more information on the original classification tree: https://data.galaxyzoo.org/gz_trees/gz_trees.html

Authors and Basic Information

- **Henry Leung** - Astronomy student, University of Toronto - henrysky
- Project advisor: **Jo Bovy** - Professor, Department of Astronomy and Astrophysics, University of Toronto - jobovy
- Contact Henry: henrysky.leung [at] mail.utoronto.ca
- This tutorial is created on 10/Feb/2018 with Keras 2.1.3, Tensorflow 1.6.0, Nvidia CuDNN 7.0 for CUDA 9.0 (Optional), Python 3.6.3 Win10 x64

This tutorial will be using astroNN

- Galaxy10 description on astroNN: http://astronn.readthedocs.io/en/latest/galaxy10.html
- astroNN github: https://github.com/henrysky/astroNN
- astroNN documentation: http://astronn.readthedocs.io/

github.com/henrysky/astroNN
github.com/henrysky/astroNN/blob/master/demo_tutorial/galaxy10/Galaxy10_Tutorial.ipynb

Neural Network for Identifying Exoplanets

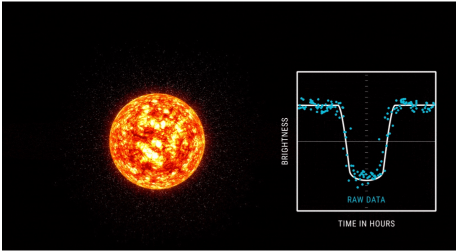
THE ASTRONOMICAL JOURNAL, 155:94 (21pp), 2018 February https://doi.org/10.3847/1538-3881/aa9e09
© 2018. The American Astronomical Society.
OPEN ACCESS

Identifying Exoplanets with Deep Learning: A Five-planet Resonant Chain around Kepler-80 and an Eighth Planet around Kepler-90

Christopher J. Shallue[1] and Andrew Vanderburg[2,3,4]
[1] Google Brain, 1600 Amphitheatre Parkway, Mountain View, CA 94043, USA; shallue@google.com
[2] Department of Astronomy, The University of Texas at Austin, 2515 Speedway, Stop C1400, Austin, TX 78712, USA
[3] Harvard–Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA
Received 2017 September 19; revised 2017 November 13; accepted 2017 November 20; published 2018 January 30

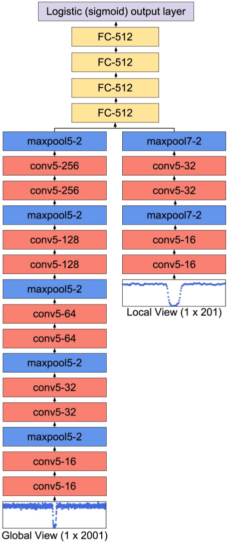
Abstract

NASA's *Kepler Space Telescope* was designed to determine the frequency of Earth-sized planets orbiting Sun-like stars, but these planets are on the very edge of the mission's detection sensitivity. Accurately determining the occurrence rate of these planets will require automatically and accurately assessing the likelihood that individual candidates are indeed planets, even at low signal-to-noise ratios. We present a method for classifying potential planet signals using deep learning, a class of machine learning algorithms that have recently become state-of-the-



Brut force training

- Data
  - 3600 planet candidates
  - 9596 astrophysical false positive
  - 2541 nontransiting phenomenon
- model
  - inputs: both global and local input
  - convolutional deep network
- training
  - Google vizier for hyper parameters tuning
  - 100 CPUs in parallel
- prediction: 10 copies model averaging



Golovin, Daniel, et al. "Google vizier: A service for black-box optimization." Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining. ACM, 2017 github.com/tobegit3hub/advisor

Astronet: Neural Network for Identifying Exoplanets

`github.com/tensorflow/models/tree/master/research/astronet`

<> Code | Issues 1,027 | Pull requests 291 | Projects 2 | Wiki | Insights

Branch: master ▾ **models / research / astronet /**

Create new file | Upload files | Find file | History

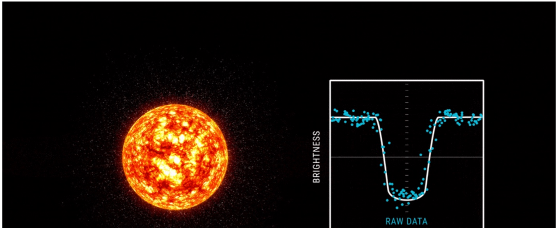
MarkDaoust Merge pull request #4629 from lamberta/fix-rename-guide-models ... Latest commit `fb3fba0` on 27 Jun

..

astronet	Update file permission mask in generate_download_script.py.	3 months ago
docs	Initial AstroNet commit.	7 months ago
light_curve_util	Add __str__ and __repr__ to periodic_event.Event.	3 months ago
third_party	Modularize light curve and TCE preprocessing functions for easier re-...	4 months ago
.gitignore	Internal change.	7 months ago
README.md	Rename programmers_guide/ to guide/ in tf-models.	3 months ago
WORKSPACE	Initial AstroNet commit.	7 months ago

README.md

AstroNet: A Neural Network for Identifying Exoplanets in Light Curves



Conclusion

- Deep learning
  - pas seulement: XGboost, SVM...
  - représentation: t-SNE
- Beaucoup de données
- Introduction d'a priori
- Attention à la méthodologie (pour bien généraliser)
- Python