An Introduction to Machine Learning **8** Astronomy Josh Peek Head of Data Science **Space Telescope Science Institute**

2024-05-20 Rare Gems 💎



John Wu



Rick White

What is Machine Learning, Anyway?





Randall Munroe, xkcd #1838



What is Machine Learning, Anyway?

"I saw the best minds of my generation solve deep, longstanding problems in Al in order to serve better ads"



~Jeff Hammerbacher, Facebook



What is Machine Learning in the astronomy context?

Machine Learning is* statistics, but where every parameter is a nuisance parameter



*(in the astronomy context)



Sometimes you want 7, sometimes you want 🙆





Ivezic, Connolly, VanderPlas & Gray 2020, astrom



What is ML in Astronomy? Supervised vs. Unsupervised Supervised Learning in Astronomy Supervised Learning: Galaxy Images Unsupervised Learning in Astronomy Unsupervised Learning: Search By Image

What is ML in Astronomy? Supervised vs. Unsupervised Supervised Learning in Astronomy Supervised Learning: Galaxy Images Unsupervised Learning in Astronomy Unsupervised Learning: Search By Image

Supervised Learning: Regression (= fitting) Classification

Unsupervised Learning: Dimensionality reduction Clustering Outlier Detection



Supervised Learning: **Regression (= fitting)** Classification

Unsupervised Learning: Dimensionality reduction Clustering **Outlier Detection**



Ivezic, Connolly, VanderPlas & Gray 2020, astroml

Classification

Supervised Learning: **Regression (= fitting)** Classification

Unsupervised Learning: Dimensionality reduction Clustering **Outlier Detection**

 $^{2}/\text{DOF} = 1.10$ 8.5 <11>e 8 0.26 7.5 log σ 6.5 $\log r_{e} (h^{3_{1}} pc, V_{INF} = 430 \text{ km/s})$ Observable Galaxy Virial Parameter Space Theorem L or R Homology, (M/L)Tĸ μ

Djorgovski & Davis 1987

Supervised Learning: **Regression (= fitting)** Classification

Unsupervised Learning: Dimensionality reduction Clustering **Outlier Detection**

Portillo+ 2020

Supervised Learning: Regression (= fitting) Classification

Unsupervised Learning: Dimensionality reduction Clustering Outlier Detection

A Brief Comment on Modality in Astronomy:

The cosmos is weakly modal compared with human experience

Supervised Learning: **Regression (= fitting)** Classification

Unsupervised Learning: Dimensionality reduction Clustering **Outlier Detection**

(a)

(c)

(b)

(d)

(h)

Segal+2023

Machine Learning has two main branches has been eaten by self-supervised learning!

Supervised Learning:

I propose an investigation into the role of dark matter mini-halos in the formation and evolution of globular clusters (GCs) in the Milky Way. This study would combine the high-precision astrometric data from Gaia EDR3 and DR3 (Gaia Collaboration et al. 2016, 2020) with spectroscopic data from large ground-based surveys like APOGEE, GALAH, SDSS SEGUE, and LAMOST to characterize the dynamics of stars in the peripheral regions of GCs. The aim would be to determine whether these GCs are embedded in dark matter mini-halos, which could provide critical insights into their origins (Peebles 1984; Peñarrubia et al. 2017). The proposed research would build upon the probabilistic approach developed by Kuzma et al. (2021) for studying the peripheral regions of GCs, which utilizes a mixture model in spatial and proper motion space to model cluster, extra-tidal, and contaminant stellar populations. By extending this approach to include the effects of dark matter mini-halos on the kinematics of stars in GC outskirts, we can test the hypothesis that dark matter plays a significant role in the formation and evolution of GCs. Furthermore, this study would provide a better understanding of the distribution and properties of dark matter in the Milky Way, contributing to the broader field of near-field cosmology. Integrating this information with the existing knowledge of the hierarchical assembly of the Milky Way (Viswanathan et al. 2023) and the role of rapid gas accretion in the inner Galactic disc (Snaith et al. 2021) would help paint a more comprehensive picture of our Galaxy's formation history and its underlying dark matter distribution.

What is ML in Astronomy? Supervised vs. Unsupervised Supervised Learning in Astronomy Supervised Learning: Galaxy Images Unsupervised Learning in Astronomy Unsupervised Learning: Search By Image

Real-Bogus: fake vs. real transients with ML

Real

Real-Bogus: Based on hand-built 30+ dimensional feature vectors

RB1

	mag	USNO-B10 derived magnitude of the candidate on the difference	e ir					
	mag err	Estimated uncertainty on mag						
	a image	Semimator axis of the candidate						
1	h image	Semiminor axis of the candidate						
•	fwhm	Full width at half-maximum (FWHM) of the candidate						
	flag	Numerical representation of the SEVTRACTOR extraction flags						
•	Ilag	Magnitude of the nearest chiest in the reference image if less then						
v	mag_rer	5 arosas from the condidate	.11					
/	mag maf and	Estimated uncertainty on man maf						
~	mag_rel_err	Estimated uncertainty on mag_rer						
	a_rei	Semimajor axis of the reference source						
~	b_rei	Semiminor axis of the reference source						
	n2sig3	Number of at least negative 2σ pixels in a 5×5 box centred on the	ie c					
	n3sig3	Number of at least negative 3σ pixels in a 5×5 box centred on the	ie c					
	n2sig5	Number of at least negative 2σ pixels in a 7×7 box centred on the	ie c					
	n3sig5	Number of at least $RB2$ \checkmark ccdid						
\checkmark	flux_ratio	Ratio of the apertur sym						
		of the reference sou 🗸 seeingnew						
	ellipticity	Ellipticity of the ca 🖌 extracted						
✓	ellipticity_ref	Ellipticity of the ref 🖌 obsaved						
\checkmark	nn_dist_renorm	Distance in arcseco pos						
	magdiff	When a reference s ✓ gauss						
		magnitude and the corr						
		Else, the difference scale						
		and the limiting ma						
1	maglim	True if there is no r 11						
	sigflux	Significance of the smooth1						
		estimated uncertain smooth2						
	seeing ratio	Ratio of the FWHN pca1						
	500116_10010	of the seeing on the pca2						
1	mag_from_limit	Limiting magnitude Test						
	normalized_fwhm	Ratio of the FWHN random						
1	normalized_fwhm_ref	Ratio of the FWHM of the reference source to the seeing in the						
	_ _	reference image						
1	good_cand_density	Ratio of the number of candidates in that subtraction to the total						
		usable area on that array						
1	<pre>min_distance_to_edge_in_new</pre>	Distance in pixels to the nearest edge of the array on the new image						

of the candidate on the difference image

pixels in a 5×5 box centred on the candidate pixels in a 5×5 box centred on the candidate pixels in a 7×7 box centred on the candidate

Numerical ID of the specific camera detector (1-12)ccdid Measure of symmetry, based on dividing the object into quadrants sym FWHM of the seeing on the new image seeingnew Number of candidates on that exposure found by SEXTRACTOR extracted Number of candidates on that exposure saved to the data base (a subset of extracted) obsaved True for a positive (i.e. brighter) residual, False for a negative (fading) one pos Gaussian best-fitting sqaured difference value gauss Gaussian best-fitting correlation value corr Gaussian scale value scale Gaussian amplitude value amp11 Sum of absolute pixel values Filter 1 output smooth1 Filter 2 output smooth2 First principal component pca1 Second principal component pca2 Zero for all candidates (i.e. no information) empty A random number generated for every candidate (i.e. pure noise) random rence source to the seeing in the

Brink + 2013

Real-Bogus: Feed these vectors to a Random Forest classifier

Images from jakevdp

A Brief Interlude on the Hegemony of Homoscedasticity

Homoscedasticity in ML and Stats: the astronomer's bane χ^2 : errors in 1DEconomicserrors in 2D

X. On the Criterion that a given System of Deviations from the Probable in the Case of a Correlated System of Variables is such that it can be reasonably supposed to have arisen from Random Sampling. By KARL PEARSON, F.R.S., University College, London*.

THE object of this paper is to investigate a criterion of the probability on any theory of an observed system of errors, and to apply it to the determination of goodness of fit in the case of frequency curves.

(1) Preliminary Proposition. Let $x_1, x_2 \ldots x_n$ be a system of deviations from the means of *n* variables with standard deviations $\sigma_1, \sigma_2 \ldots \sigma_n$ and with correlations $r_{12}, r_{13}, r_{23} \ldots r_{n-1, n}$.

Then the frequency surface is given by

$$-\frac{1}{2} \left\{ S_1 \left(\frac{R_{pp}}{R} \frac{x_p^2}{\sigma_p^2} \right) + 2S_2 \left(\frac{R_{pq}}{R} \frac{x_p}{\sigma_p} \frac{x_q}{\sigma_q} \right) \right\}$$

$$Z = Z_0 e \qquad , \dots (i.)$$

where R is the determinant

1	r_{12}	$r_{13} \cdot \cdot \cdot r_{1n}$
r_{21}	1	$r_{23}\ldots r_{2n}$
r_{31}	r_{32}	$1 \dots r_{3n}$
• •		
		• • · ·
r _{n1}	r_{n2}	r_{n3} 1

and R_{pp} , R_{pq} the minors obtained by striking out the *p*th row and *p*th column, and the *p*th row and *q*th column. S_1 is the sum for every value of *p*, and S_2 for every pair of values of *p* and *q*.

Now let

$$\chi^2 = S_1 \left(\frac{R_{pp}}{R} \frac{x_p^2}{\sigma_p^2} \right) + 2S_2 \left(\frac{R_{pq}}{R} \frac{x_p x_q}{\sigma_p \sigma_q} \right) \cdot \cdot \cdot \cdot (ii.)$$

Then: $\chi^2 = \text{constant}$, is the equation to a generalized "ellipsoid," all over the surface of which the frequency of the system of errors or deviations $x_1, x_2 \ldots x_n$ is constant. The values which χ must be given to cover the whole of space are from 0 to ∞ . Now suppose the "ellipsoid" referred to its principal axes, and then by squeezing reduced to a sphere, $X_1, X_2, \ldots X$ being now the coordinates; then the chances of a system of errors with as great or greater frequency than

12 34

Pearson 1900

Everyone, entirety of 20th c.

Hogg, Bovy, & Lang 2010

Homoscedasticity in ML and Stats: the astronomer's bane Economics **Probabilistic RF Random Forest**

Everyone, forever, apparently

Reis, Baron, & Shahaf 2017

A Brief Interlude on the Hegemony of Homoscedasticity

Astronomers cannot rely on the ML community, we must join it!

Neural Networks are actually pretty simple*

Neural Networks are actually pretty simple

Neural Networks are actually pretty simple

Neural Networks are actually pretty simple

Deep Neural Networks use Many Hidden Layers; hard for many inputs

Weights \propto # neuron^2 x # layers \Im

Convolutional Neural Networks (CNNs) are designed for images

scs.rye	erson.ca		C			ÓÍ	1 O	+
01234	456789							

A Brief Interlude on image information:

Pixel-driven ML (e.g. neural nets) impose many fewer assumptions about where the information is

Astronomers know how to look at the sky in 3 ways

Astronomers know how to look at the sky in 3 ways

any image

is this a Gaussian Random Field?

Power Spectra

any image is this a bunch of points?

Black-Sky Segmentation

CNNs can extract shape information from Weak Lensing maps

CNNs can extract masses from galaxy clusters by excising cores

feature extraction

i.5 2.0 ≤1.0 log(N)

Ntampaka +2019

Networks don't have to be in the abstract

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The DECam Plane Survey: Optical Photometry of Two Billion Objects in the Southern **Galactic Plane**

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Abstract

The DECam Plane Survey is a five-band optical and near-infrared survey of the southerr Dark Energy Camera at Cerro Tololo. The survey is designed to reach past the mainpopulations at the distance of the Galactic center through a reddening E(B - V) of exposure depths are 23.7, 22.8, 22.3, 21.9, and 21.0 mag (AB) in the grizY bands, wit footprint covers the Galactic plane with $|b| \leq 4^{\circ}$, $5^{\circ} > l > -120^{\circ}$. The survey pipeline s the positions and fluxes of tens of thousands of sources in each image, delivering positio two billion stars with better than 10 mmag precision. Most of these objects are highly r Galactic disk, probing the structure and properties of the Milky Way and its interste processed images and derived catalogs are publicly available.

Key words: catalogs – surveys – techniques: photometric

1. Introduction

Many of the Milky Way stars and much of its gas and dust reside in a disk. Accordingly, observations of the Milky Way disk are critical to understanding the Milky Way-particularly observations toward the inner Galaxy, where most of the mass lies. At optical wavelengths, however, the interpretation of observations of the Milky Way disk can be challenging due to the tremendous number of stars and due to extinction by dust, motivating surveys of the disk at infrared wavelengths where autination is greatly radiused

photometric measurements of of data for understanding the

DECaPS occupies a specia targeting the Milky Way. Th PS1 survey (Chambers et al. very similar set of filters and is roughly 1 mag deeper in i covers the entire sky abov epochs than DECaPS does valuable survey for understa



https://doi.org/10.3847/1538-4365/aaa3e2



Page 4

Schlafly_2018_ApJS_234_39.pdf

3 matches

Convolutional neural networks (CNNs) are ide...



Page 5

10 matches

We used 80% of the images to train the netw...







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Morphology is a key weapon in the physicist's arsenal

Scheme



Galaxy Zoo took morphology to the big data era













Now we can study morphology like color



Bamford + 2009



Machine Learning let us take the next jump



This is the starting gun of deep learning in astro











Dieleman+2015







Images contain information about metallicity

	Lowest Z _{pred}				*
(a)			1		
	$Z_{true} = 8.153$ $Z_{pred} = 8.130$	$Z_{true} = 8.212$ $Z_{pred} = 8.162$	$Z_{true} = 8.204$ $Z_{pred} = 8.177$	$Z_{true} = 7.997$ $Z_{pred} = 8.181$	$Z_{true} = 8.308$ $Z_{pred} = 8.187$
	Lowest Z _{true}				
(b)					•
	$Z_{true} = 7.896$ $Z_{pred} = 8.211$	$Z_{true} = 7.959$ $Z_{pred} = 8.211$	$Z_{true} = 7.976$ $Z_{pred} = 8.467$	$Z_{true} = 7.997$ $Z_{pred} = 8.181$	$Z_{\text{true}} = 8.010$ $Z_{\text{pred}} = 8.647$
	Highest Z _{pred}				
(c)			5		
	$Z_{true} = 9.211$ $Z_{pred} = 9.200$	$Z_{true} = 9.325$ $Z_{pred} = 9.182$	$Z_{\text{true}} = 9.264$ $Z_{\text{pred}} = 9.181$	$Z_{true} = 9.095$ $Z_{pred} = 9.181$	$Z_{true} = 9.466$ $Z_{pred} = 9.180$
(d)	Highest Z _{true}				
				•	
	$Z_{true} = 9.466$ $Z_{pred} = 9.180$	$Z_{true} = 9.461$ $Z_{pred} = 9.158$	$Z_{true} = 9.432$ $Z_{pred} = 9.029$	$Z_{true} = 9.406$ $Z_{pred} = 9.060$	$Z_{\text{true}} = 9.405$ $Z_{\text{pred}} = 8.916$
j	Most underpredicted				
(e)					
(0)				10 A 10	
	$Z_{true} = 9.405$ $Z_{pred} = 8.916$	$Z_{true} = 9.336$ $Z_{pred} = 8.888$	$Z_{\text{true}} = 8.932$ $Z_{\text{pred}} = 8.495$	$Z_{true} = 9.290$ $Z_{pred} = 8.859$	$Z_{\text{true}} = 8.870$ $Z_{\text{pred}} = 8.456$
	Most overpredicted	C. Salar			- Children
(f)				•	
	$Z_{true} = 8.248$ $Z_{pred} = 9.103$	$Z_{true} = 8.363$ $Z_{oved} = 9.057$	$Z_{true} = 8.312$ $Z_{pred} = 8.995$	$Z_{\text{true}} = 8.010$ $Z_{\text{pred}} = 8.647$	$Z_{true} = 8.293$ $Z_{pred} = 8.927$
	Random				
(a)					
(9)					
	$Z_{true} = 8.747$ $Z_{pred} = 8.759$	$Z_{true} = 9.130$ $Z_{pred} = 9.093$	$Z_{\text{true}} = 9.131$ $Z_{\text{pred}} = 9.125$	$Z_{true} = 8.768$ $Z_{pred} = 8.763$	$Z_{true} = 8.861$ $Z_{pred} = 8.735$



Networks can tell us how they know something physical

AGC 8056	gas-poor	gas-rich	AGC 723474	gas-poor	gas-rich
	p = 0.003	ρ = 0.997		p = 0.048	p = 0.952
a)	p = 0.082	p = 0.918	b)	p = 0.104	p = 0.896
AGC 220300	gas-poor $p = 0.514$	gas-rich 000000000000000000000000000000000000	AGC 221013	gas-poor <i>p</i> = 0.949	gas-rich $p = 0.051$
C)	p = 0.813	p = 0.187	d)	p = 0.877	p = 0.123

Wu 2020



Networks can tell us how they know something physical



Wu 2020



Cut to the chase: the entire spectrum from the image







Wu & JEGP 2020





Cut to the chase: the entire spectrum from the image







A practical example: finding low-z galaxies

SAGA is the premier spectroscopic survey of low-z satellites378+ new satellites around 101 hosts, using > 75,000 spectraGeha+ 17, Mao+21, Mao+24



A CNN robustly selects low-z galaxies

SAGA training sample





A CNN robustly selects low-z galaxies

SAGA training sample



xSAGA test sample

Wu, JEGP+ 22



CNN is ~15x better than photo selection tested nightly on DESI



Darragh-Ford, Wu, + JEGP + 22













Legacy Survey grz





HSC Survey grz (similar to LSST)





Hubble F606W/F814W (similar to Roman)

We are just getting started...



100

What is ML in Astronomy? Supervised vs. Unsupervised Supervised Learning in Astronomy Supervised Learning: Galaxy Images Unsupervised Learning in Astronomy Unsupervised Learning: Search By Image

Why Unsupervised (or Self-Supervised) Learning?

hypothesis generation in the big data era is an unsolved problem



Finding the *weirdest* Galaxies in SDSS spectra





2e6 de-redshifted spectra with 15000 "features"

Random Forest to find similarity: how often in the same leaf?



Weirdness score: on average how far from every other galaxy?

Baron & Poznanski 2017





Detailed studies with KCWI show an E+A galaxy with AGN winds







110 to 210 km/s



0









20

15-













320 to 430 km/s









All galaxies are public, but few have been explored



Roct wavelength [A]

http://galaxyportal.space, Reis+ 2018

 \mathbf{v}

Order



We also need big data discovery beyond outliers: gaps

A GAP IN MAIN SEQUENCE



Jao+ 2018, Contardo, Hogg, Hunt, JEGP, Chen ,2022



But: Machine Learning is also a stumbling block



Zucker, JEGP, & Loebman 2022; Powered by SciX



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How do you find data in an archive?

NASA science image archives allow users to find images by metadata:

What camera, filter, exposure time, PI, position?

Catalogs of the objects contained in those images provide a limited search of the data itself:

Find images containing objects of a given brightness, position, basic shape ...

We are developing tools to answer a much harder question:

If I have a complex image, how can I find all the images in the archive that look like it?





Found in the HST archive today: a nice example of an X-shaped boxy bulge galaxy. This is IC 2059, from program 14840, the original pilot gap-filler program. Similar to the structure of NGC 1175.















Image

Cutouts

Existing Network



Feature Vector

Clustered data





Carina Image







Carina Image







Carina Image





JEGP+ 2020


Search by Image: a problem with many approaches for many sciences



Self-Supervised Learning is a generic approach to unlabeled data:

Modify images through rotation, stretch, cropping, and associate them to each other.

Earth Science is interested in similar problems with unlabeled data:

Finding hurricanes, wildfires, ice movement, etc

SpaceML is a team of industry professionals working with Earth Science on DL approaches

We teamed up with SpaceML to test SSL approaches and provide verification data sets





How do we optimize this approach? Which way is best?

We need a sample of images with known similarities to test, improve, and compare our algorithms!

The Hubble and Planetary Image Similarity Projects (HISP/PISP)

HISP and PISP aims to create a large database of similarity information of Mars Reconnaissance Orbiter (CTX).

- The images are compared by humans in a citizen science project.
- We also designed the project for community impact:
 - We employ service-industry professionals from the local area near STScl in Baltimore who were impacted by the Covid-19 pandemic.
 - They are paid a fair wage for their work through the Amazon Mechanical Turk (AMT) system.

between segments of Hubble images (ACS & WFC3) and between segments

White & JEGP in prep







Elliptical NGC object



Elliptical NGC object HST WFC3/UVIS footprint



Elliptical NGC object HST WFC3/UVIS footprint 488x488 pixel cutout images



Elliptical NGC object HST WFC3/UVIS footprint 488x488 pixel cutout images



Elliptical NGC object HST WFC3/UVIS footprint 488x488 pixel cutout images



























Sample includes nebulae, clusters, star formation regions









Image entropy selects cutouts with good contrast



Select similar images from the Hubble Space Telescope

Comparison image

Comparison image

Which of these **15 images** *are similar* to the **Comparison Image** at left?







Submit

Select similar images from the Mars Reconnaissance Orbiter

Comparison image

Which of these 15 images are similar to the Comparison Image at left?



Submit

No images are similar

Submit

Submit



IC4641 (-2.5,-33.9) 0.000



NGC3982 (-1.4,-34.5) 1.213



NGC3949 (-1.8,-32.8) 1.300



NGC4625 (-3.2,-32.5) 1.573



NGC3021 (-1.7,-33.4) 0.897



NGC7823 (-3.2,-34.9) 1.243



NGC3310 (-3.8,-34.3) 1.376



NGC4800 (-0.9,-34.4) 1.600



NGC3278 (-1.8,-33.1) 1.058



NGC2255 (-1.7,-34.9) 1.259



NGC4940 (-1.1,-34.3) 1.417



NGC4790 (-3.1,-35.4) 1.671













NGC3433 (-0.8,-5.8) 0.000



NGC6557 (-2.1,-5.4) 1.344



NGC0266 (-0.1,-4.0) 1.868



NGC5448 (-2.6,-4.3) 2.348



NGC7407 (-0.8,-5.4) 0.378



NGC5064 (-2.1,-6.3) 1.419



NGC0986 (-2.2,-7.1) 1.935



NGC0634 (-1.3,-8.3) 2.552



NGC0289 (-0.4,-6.6) 0.908



NGC3145 (-2.2,-6.9) 1.804



NGC0634 (-0.1,-7.8) 2.159



NGC5985 (-1.9,-3.4) 2.584













NGC7541 (-8.5,-20.7) 0.000



NGC5010 (-8.7,-22.7) 2.032



NGC7130 (-10.1,-18.7) 2.499



NGC4496A (-10.9,-19.0) 2.862







NGC2748 (-7.4,-18.7) 2.285



NGC2748 (-7.5,-18.3) 2.559



NGC5714 (-8.2,-23.6) 2.911



NGC3370 (-9.5,-19.5) 1.516



NGC4634 (-6.5,-19.7) 2.288



NGC3287 (-8.3,-18.0) 2.666



IC1127 (-6.0,-19.2) 2.971













NGC3603 (3.5,16.2) 0.000



NGC3603 (3.3,15.4) 0.887



NGC3603 (4.6,15.3) 1.411



NGC2060 (2.6,17.5) 1.593



NGC3603 (3.2,16.3) 0.342



NGC6357 (4.3,16.8) 0.995



NGC2078 (2.8,15.0) 1.455



NGC3603 (4.1,14.6) 1.723



NGC3603 (3.9,15.7) 0.639



NGC3603 (2.5,15.9) 1.124



NGC3603 (3.7,14.7) 1.523



NGC2078 (2.9,14.6) 1.725















The Self-Supervised Learning approach works!



Walker Stevens for the SpaceML team

Conclusions:

Conclusions: Machine Learning is a popular and powerful tool for astronomy, but not a replacement for statistics

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Conclusions: Machine Learning is a popular and powerful tool for astronomy, but not a replacement for statistics Astronomers need to join with ML experts to develop tools appropriate for astronomical problems We have gone from morphological classification to true physical analyses with deep learning on galaxy images and we are just getting started Hypothesis generation in the big data era is still an unsolved problem in astronomy **Cross-industry and cross-science deep learning** approaches will create new tools for astroinformatics in the 2020s







