

La inteligencia artificial como soporte a decisiones

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MINISTERIO
DE CIENCIA, INNOVACIÓN
Y UNIVERSIDADES

Ciemat

Centro de Investigaciones
Energéticas, Medioambientales
y Tecnológicas

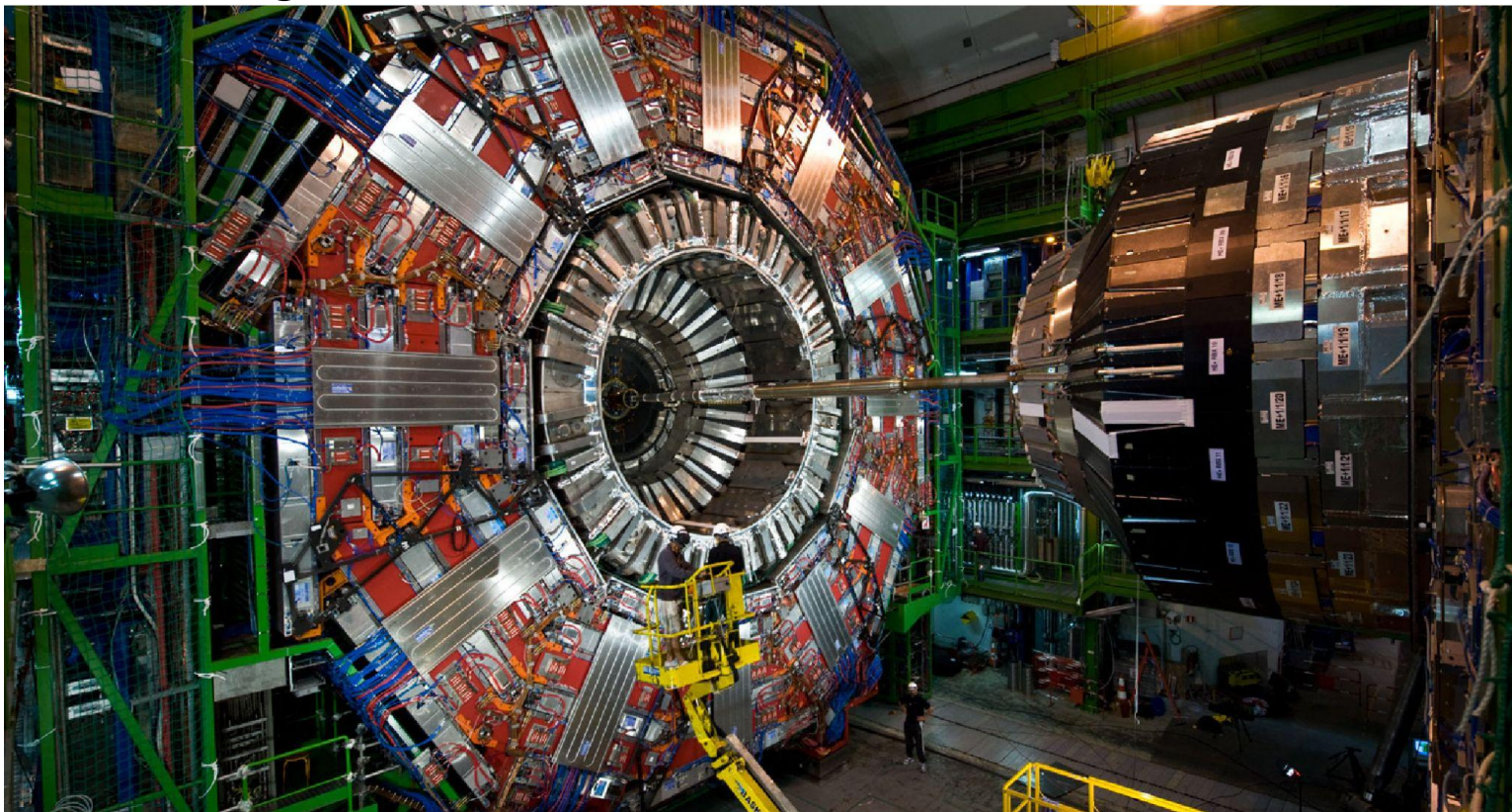
SERVICIOS INNOVADORES DE ANÁLISIS DE DATOS PARA EL EXPERIMENTO CMS. **PID2020-113807RA-I00**

CIEMAT



CIEMAT - Investigación Básica

CMS



CIEMAT - Investigación Básica

AMS



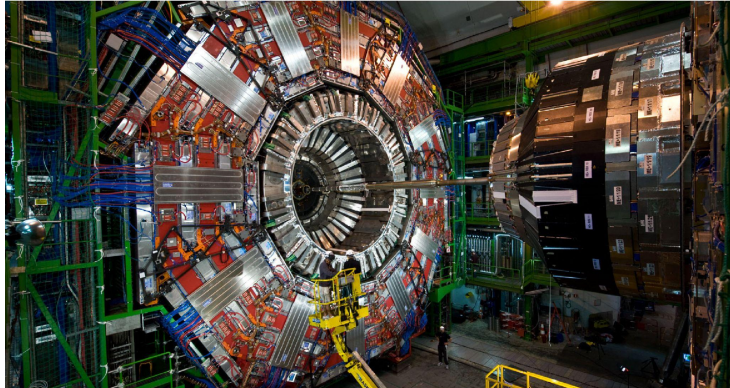
CIEMAT - Investigación Básica

CTA



Dept. Investigación Básica

- La Física más allá del Modelo Estándar.
- ¿Son los neutrinos una ventana a nueva física?
- La naturaleza de la Materia Oscura.
- La naturaleza de la Energía Oscura.
- Gran actividad tecnológica: ingeniería mecánica, electrónica e informática.



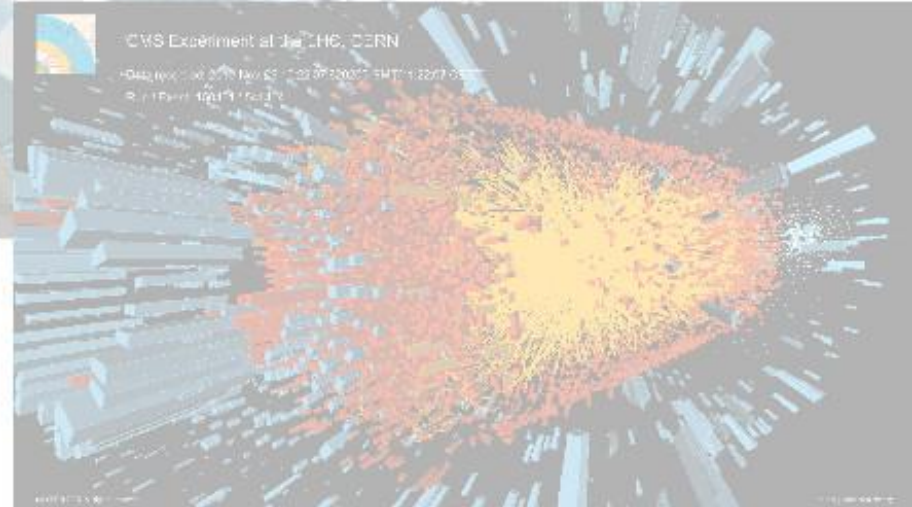
Big Data en Ciencia

- LHC, O(20 PB/año), 1 dispositivo.

Incremento en un orden de magnitud a partir de +2025.

¿Es posible incrementar el presupuesto de computación científica en la misma proporción?

- LSST, O(12 PB/año), 1 dispositivo
- NGS (secuenciación masiva de genes),
O(0.5 TB/genoma),
O(1/hospital) dispositivos.

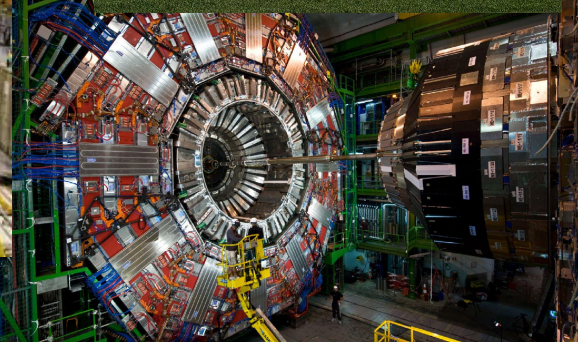


Sensorización: volumen, velocidad, variedad, v's...

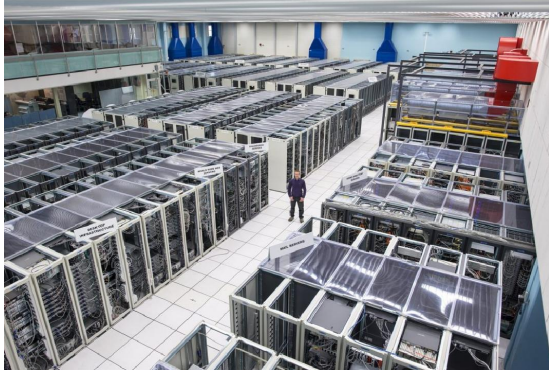
El incremento en la sensorización en los detectores (y dispositivos industriales) conduce a un incremento del **volumen de datos**, su **velocidad de generación** y la **variedad de formatos y fuentes**.

Detectores y sus entornos con mayor densidad de sensores con más velocidad.

Nuevos desafíos: **procesar más rápido**, sobre **más datos de mayor complejidad** y con menor huella de carbono.

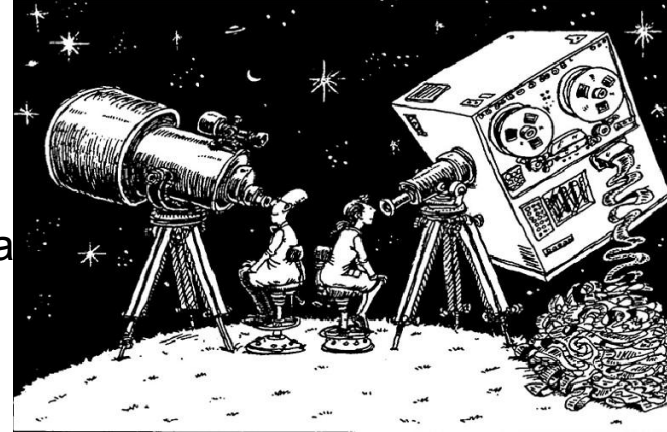


Barreras para el mantenimiento de la producción científica



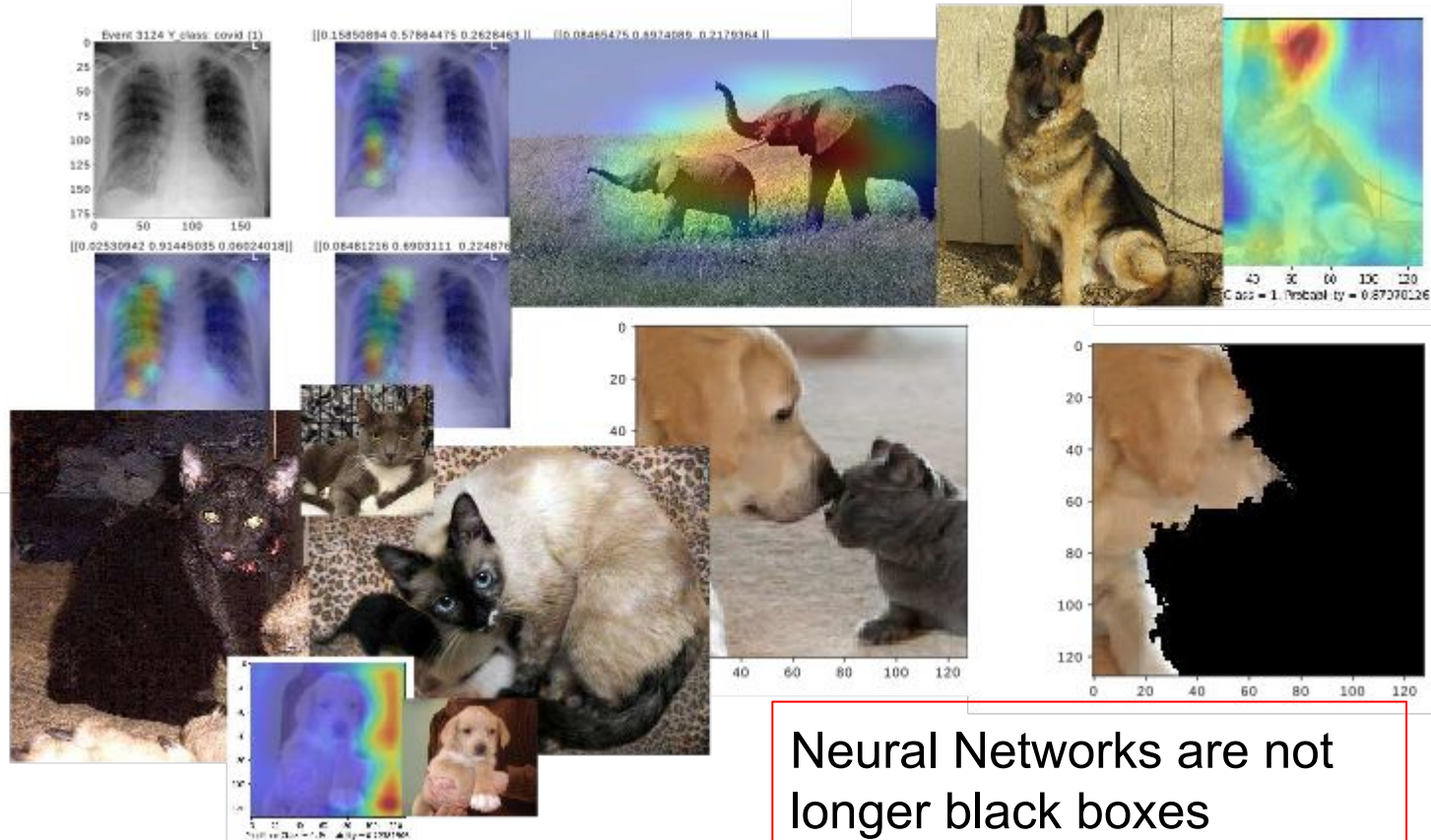
- **Extracción de información.**

- Gestión de datos: hacer los datos disponibles a los científicos.
- Tiempo de procesamiento.
- Debilidades de la representación numérica.



eXplainable Artificial Intelligence XAI

XAI, intuition



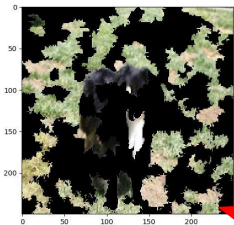
Neural Networks are not
longer black boxes

XAI, intuition and biased learning

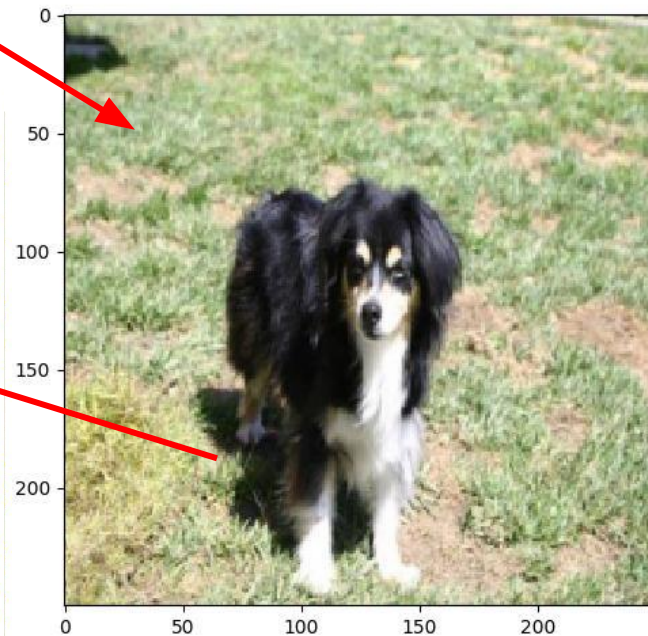
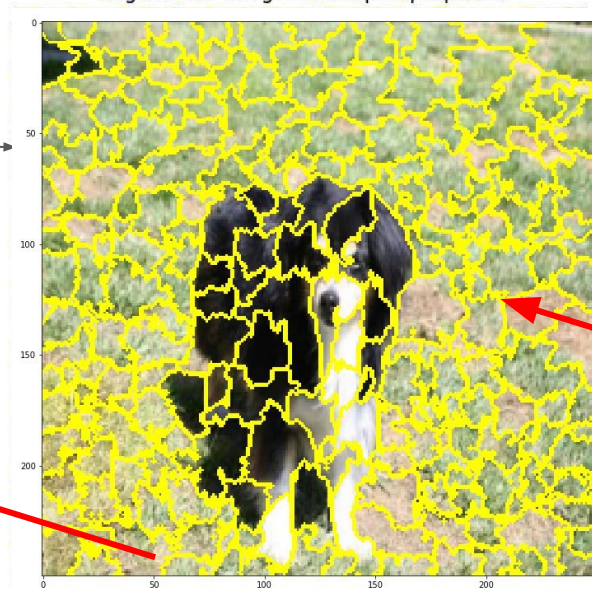
Dog correctly classified as dog (class 1): $[4.8\text{e-}11$ (cat), $1.0\text{e+}00$ (dog)]

Image segmented in homogeneous patches (~250).

Randomly patches are switched on/off and then predicted.



Segmented Image with Top Superpixels



Degradation of prediction illuminates the importance of the patches. And repeat ...

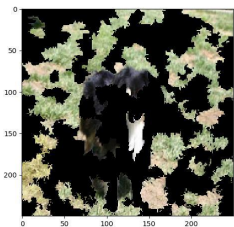
Linear regressor with patches on/off as input and the performance degradation as output.

XAI, intuition and biased learning

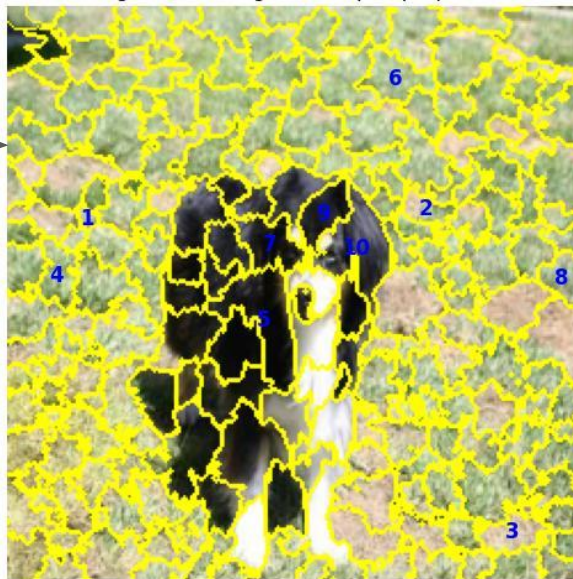
Dog correctly classified as dog (class 1): [4.8e-11 (cat), 1.0e+00 (dog)]

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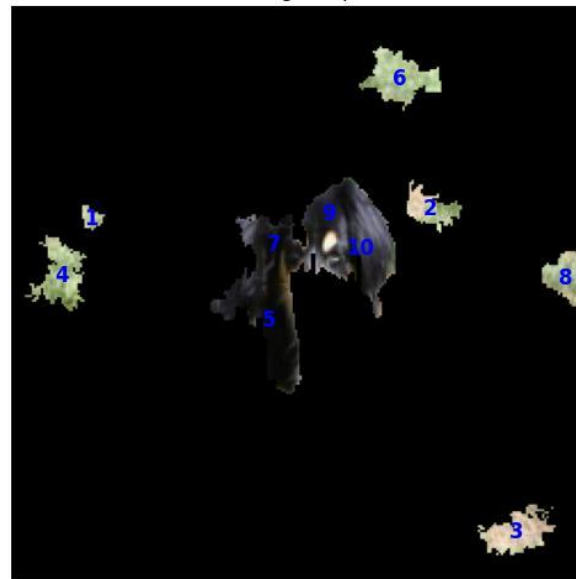


Segmented Image with Top Superpixels



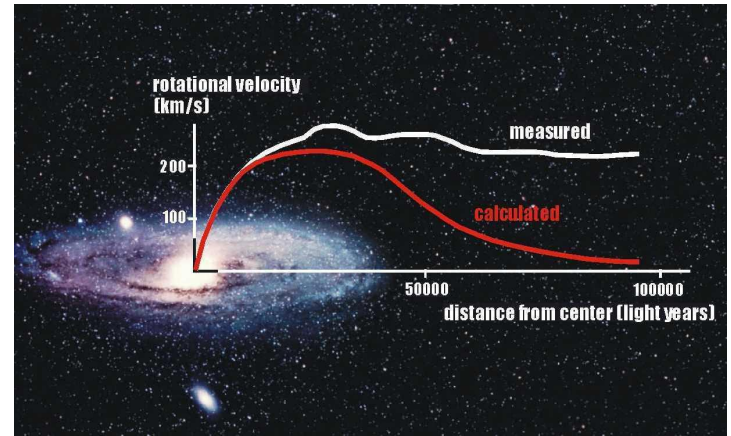
The 10 most important patches are mostly **grass**.

Perturbed Image (Top Features)



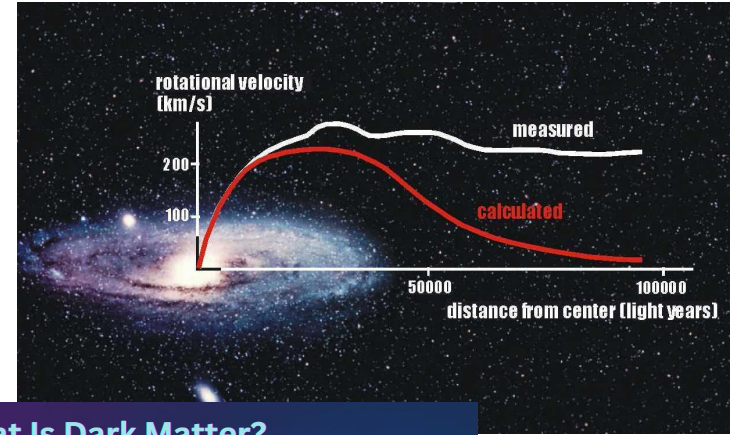
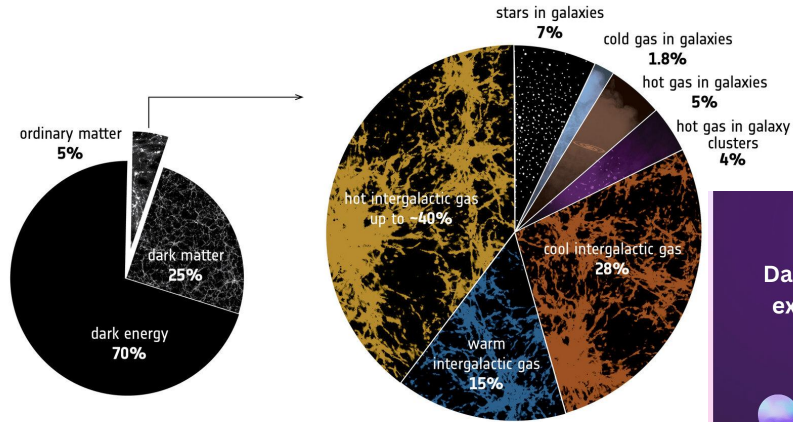
Degradation of prediction illuminates the importance of the patches. And repeat ...

Linear regressor with patches on/off as input and the performance degradation as output.



DEAP-3600 y búsqueda de Materia Oscura

Materia Oscura



What Is Dark Matter?

Dark matter is a hypothetical form of invisible matter that exerts gravitational effects on light and ordinary matter.

axion

gravitino

?

Dark Matter

neutron

antimatter

neutrino

proton

Visible Matter

electron

WIMP

neutralino

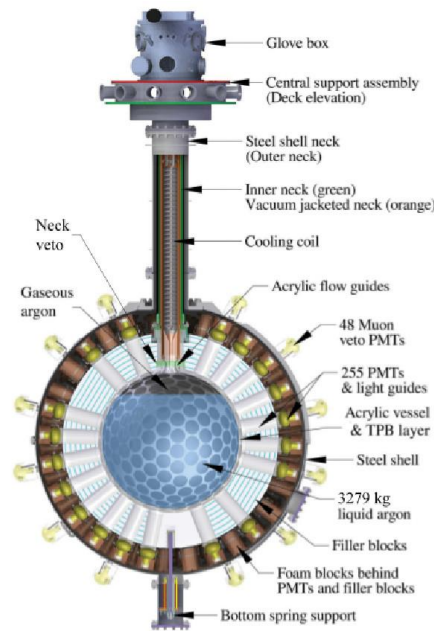
?

The Universe consists of 5% matter, 27% dark matter, and 68% dark energy.

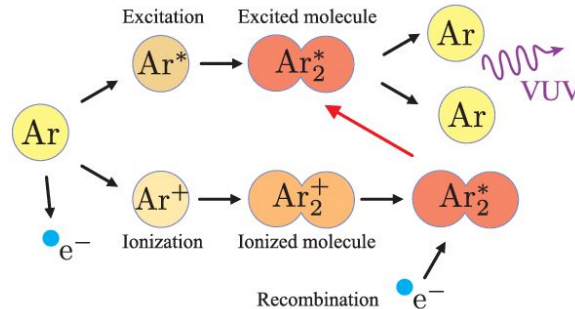
sciencenotes.org

DEAP-3600

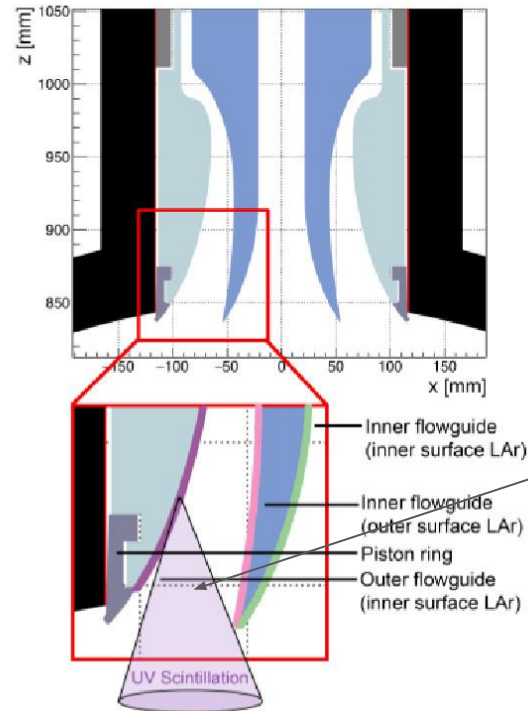
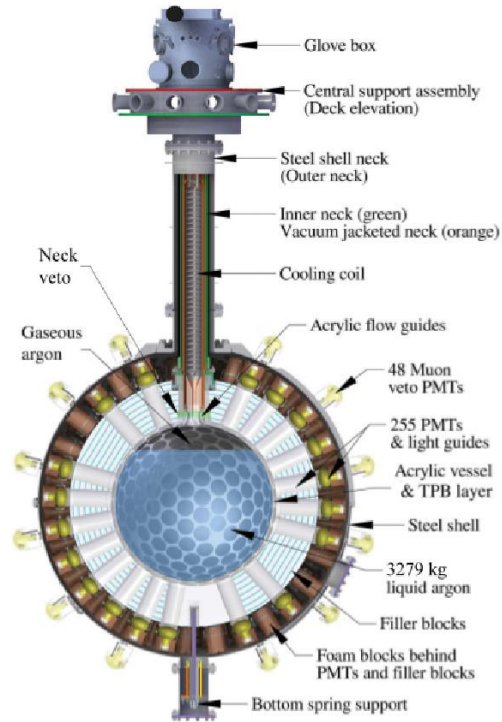
- Placed in SNOLAB under 2 km of rock (≈ 6000 mwe of coverage).
- Spherical acrylic vessel with diameter of 170 cm. It is filled with 3279 kg Liquid Argon.
- Single phase detector with 255 PMTs covering the 75% of the sphere. Grouped in 35 rings: 5 or 10 PMTs



¿Podemos hacer un buen trabajo en análisis de datos sin entender cómo se originan?



α Cuello en DEAP-3600

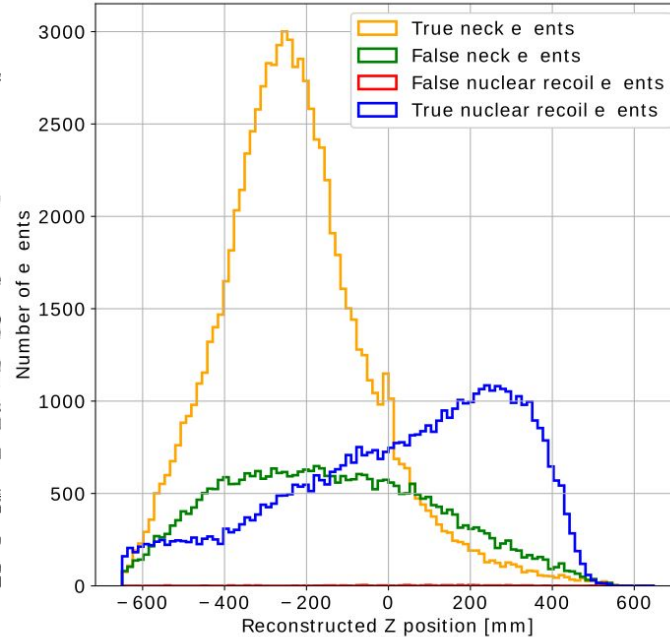
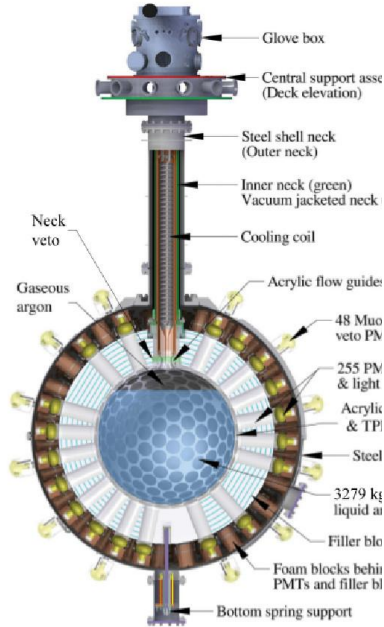


En 2018, α cuello es el fondo dominante.

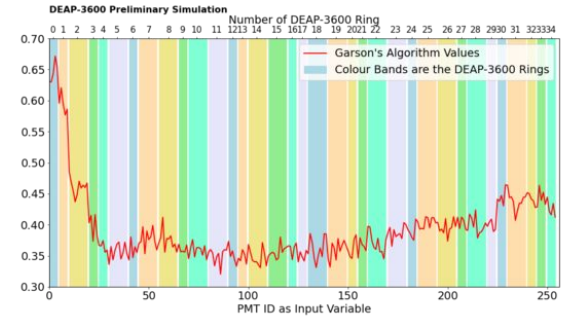
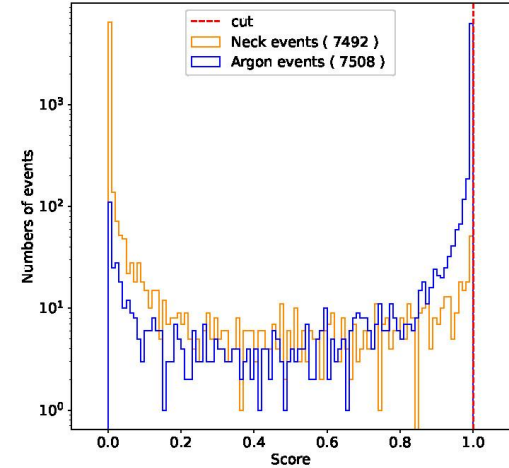
α centellea en LAr condensado sobre las guías de luz.

Topológicamente colimado: empuja evento al hemisferio sur.

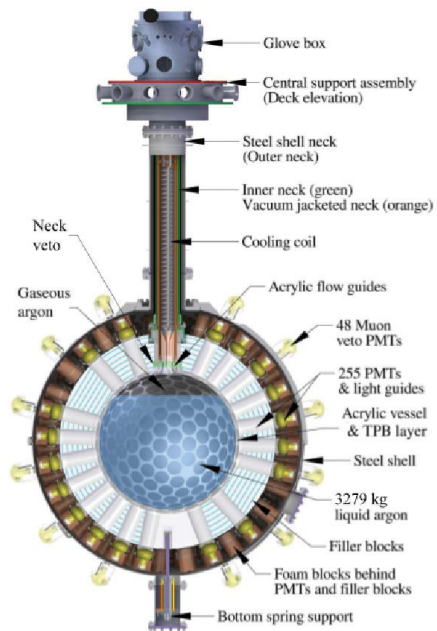
α Cuello en DEAP-3600: MLP



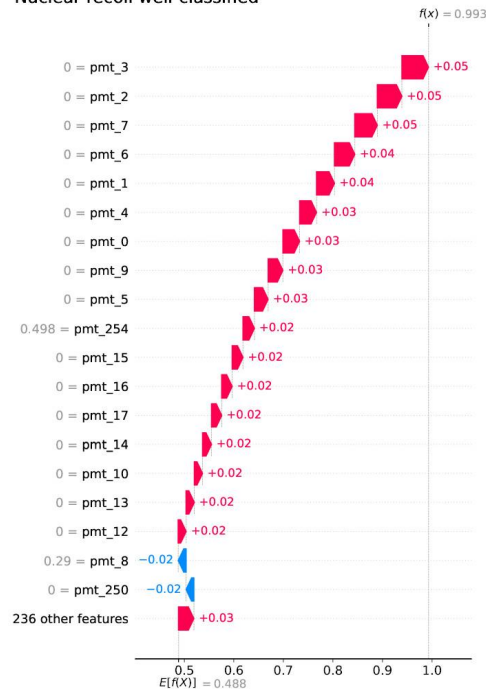
DEAP – 3600 Preliminary Simulation
Neck- α misclassified



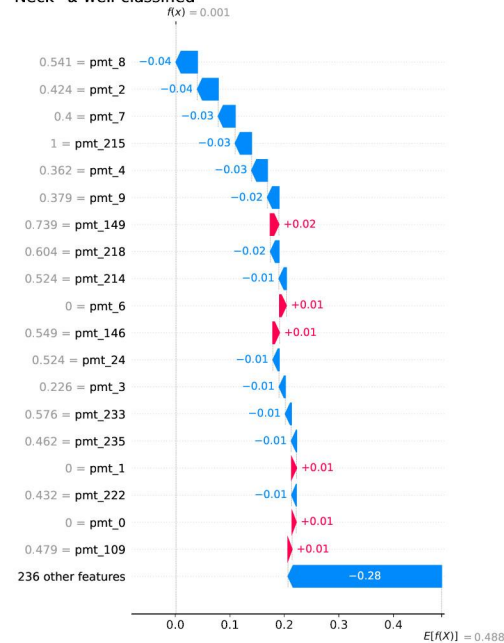
α Cuello en DEAP-3600: MLP



DEAP – 3600 Preliminary Simulation
Nuclear recoil well-classified



DEAP – 3600 Preliminary Simulation
Neck- α well-classified



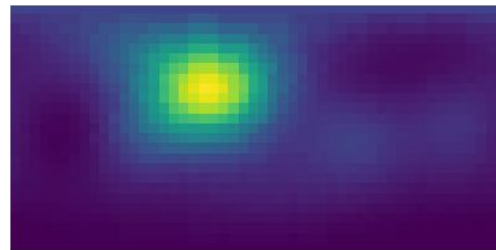
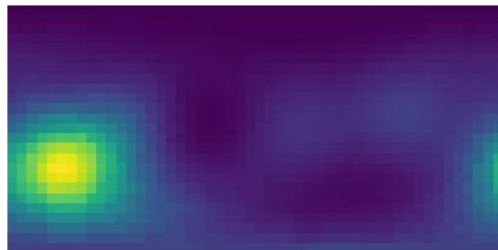
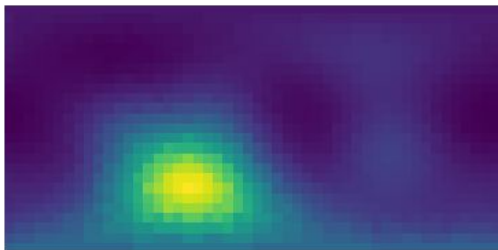
Eventos en imágenes realistas

Vista frontal

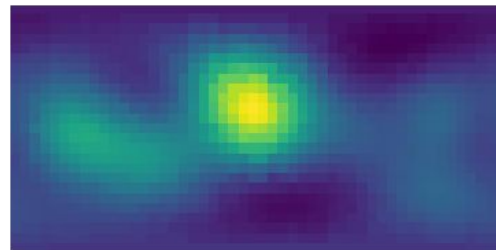
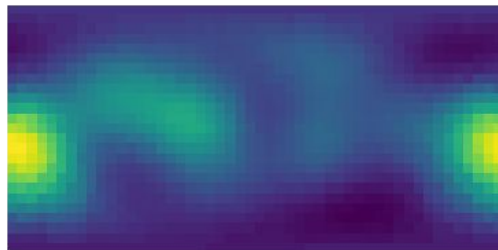
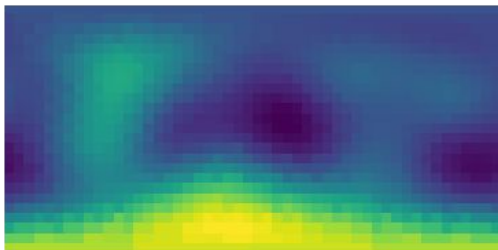
Vista superior

Vista inferior

HEALPix



retroceso
nuclear



cuello

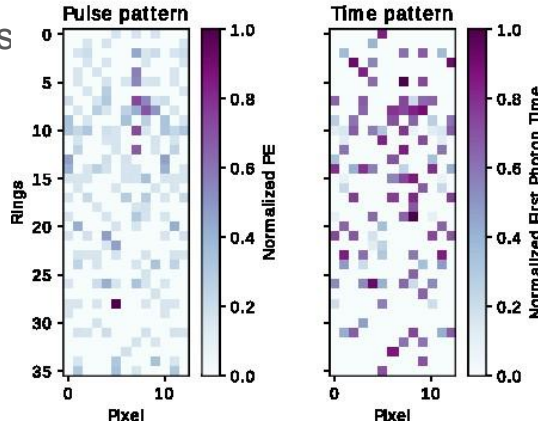
- 60 Kbytes por imagen, $\times 0.5 \cdot 10^6$ imágenes $\approx 10^7$ Kbytes, 10Gbytes.
- 10 s por trío de imágenes $\times 0.5 \cdot 10^6$ imágenes $\approx 10^7$ s, 2777h, 115d

Buena idea, pero mal ejecutada.

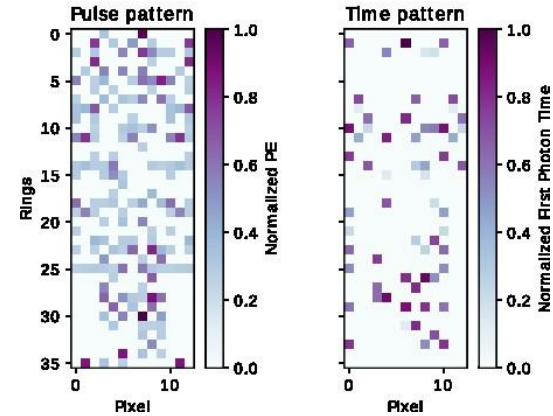
Imágenes de eventos

- Creación de imágenes rectangulares
- Anillos con 5 o 10 fotomultiplicadores (relleno con píxeles nulos en los anillos de 5 fotomultiplicadores).
- Patrón de luz y patrón de tiempo usando una pseudo imagen. 2 canales.
- Repetición de las primeras 3 columnas.
- Explotación de la correlación entre píxeles en los patrones de luz y tiempo mediante CNN2D.

DEAP - 3600 Preliminary Simulation
Nuclear recoil R = 650 mm



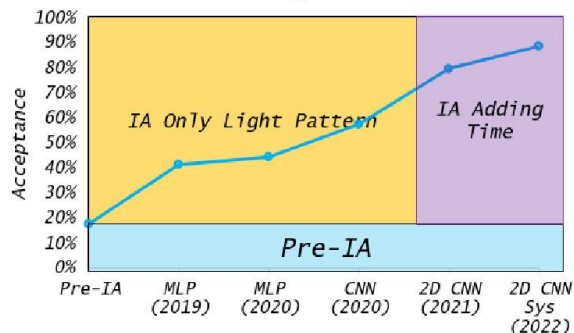
DEAP - 3600 Preliminary Simulation
Neck- α



Imágenes de eventos

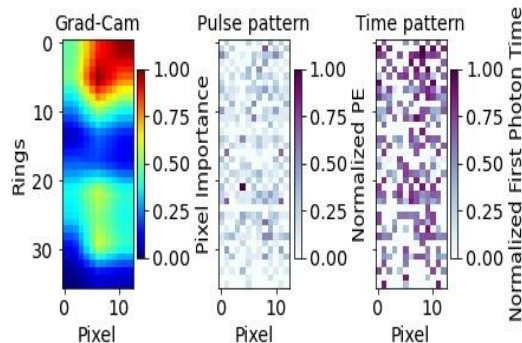
- Con estas mejoras la **aceptancia** alcanzó un 80% para un **poder de rechazo** del 99.9%.

Evolution of Acceptance for 99.9% rejection



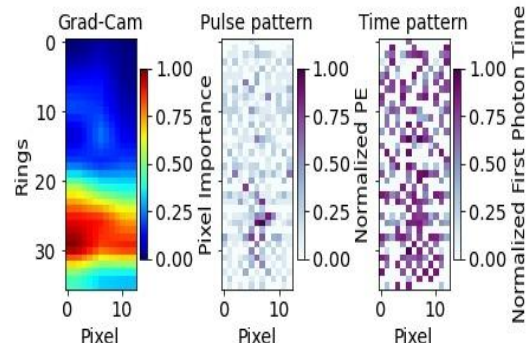
DEAP – 3600 Preliminary Simulation

Neck $-\alpha$

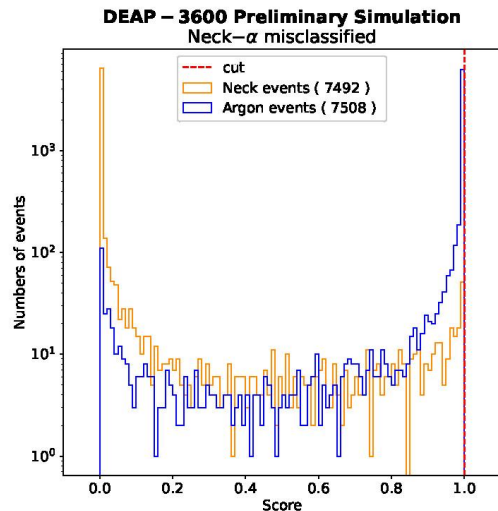


DEAP – 3600 Preliminary Simulation

Nuclear Recoil R = 606 mm



α Cuello en DEAP-3600: loss

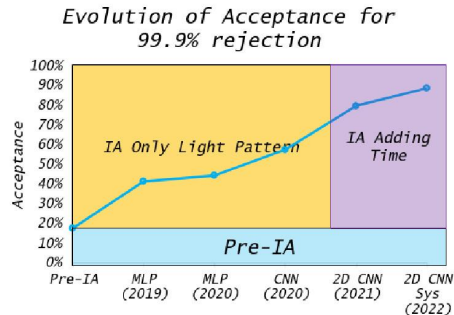
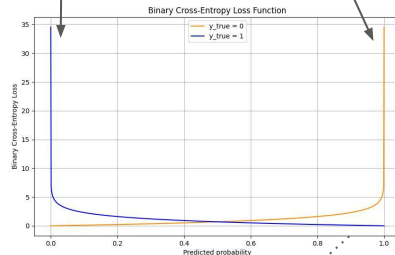


Aceptancia x5
Rechazo x10

Aceptancia: 36% -> 90%

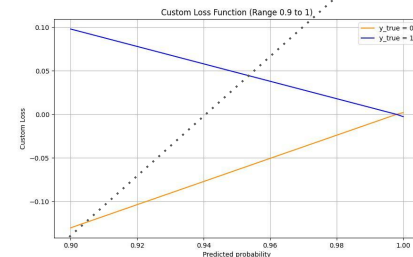
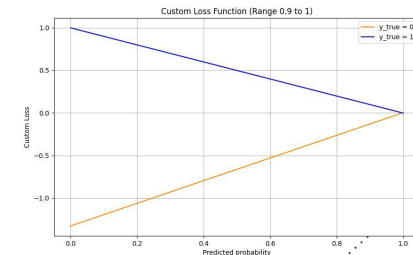
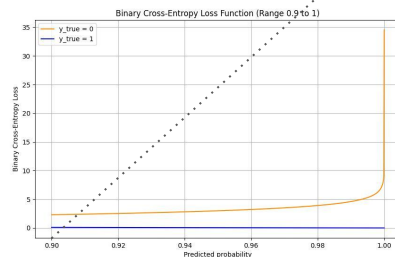
$$H_p(q) = -\frac{1}{N} \sum_{i=1}^N y_i \cdot \log(p(y_i)) + (1 - y_i) \cdot \log(1 - p(y_i))$$

Binary Cross-Entropy / Log Loss

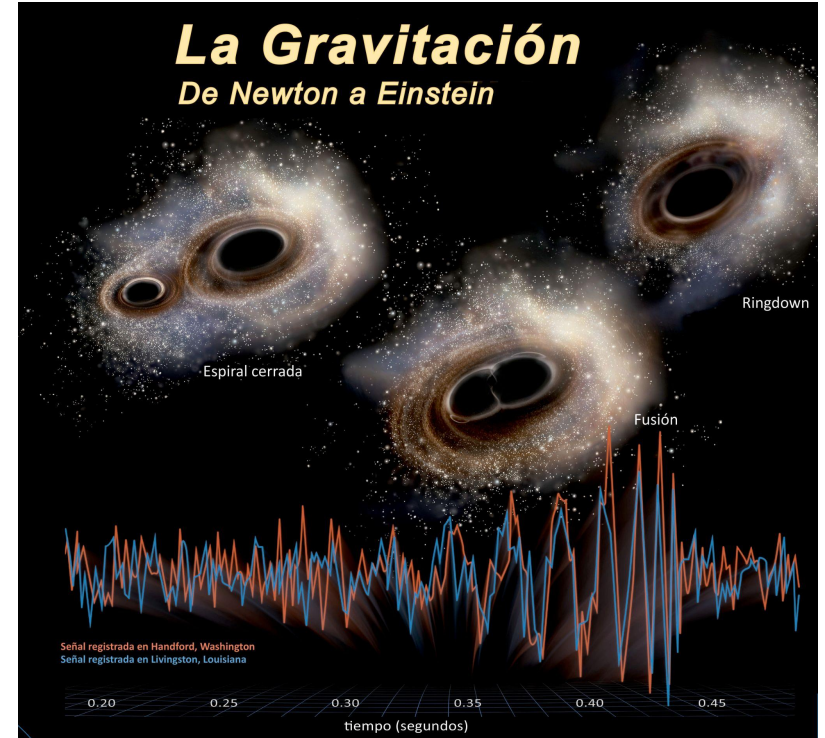


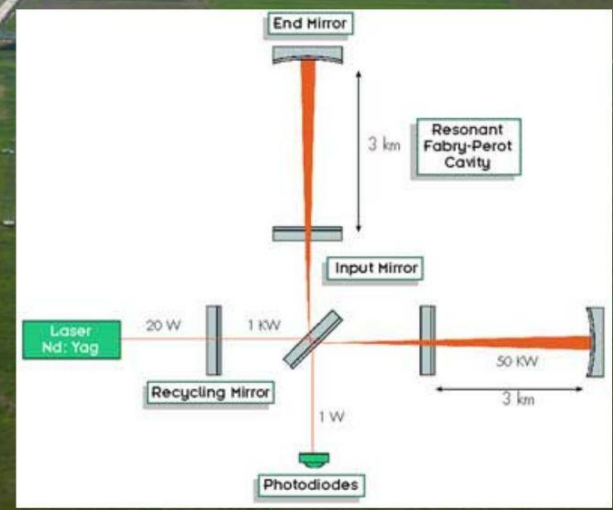
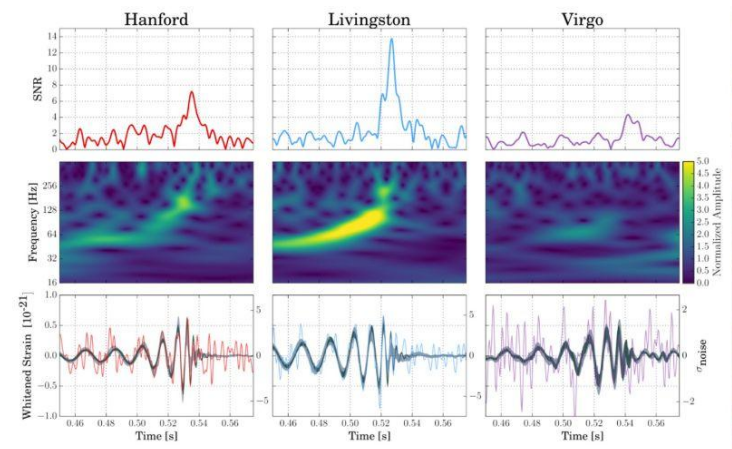
Ciclo virtuoso con NN:

1. Más parámetros entrenables
2. XAI-> qué aprenden las NN
3. Formato de datos
4. Función Error personalizada



Ondas Gravitacionales

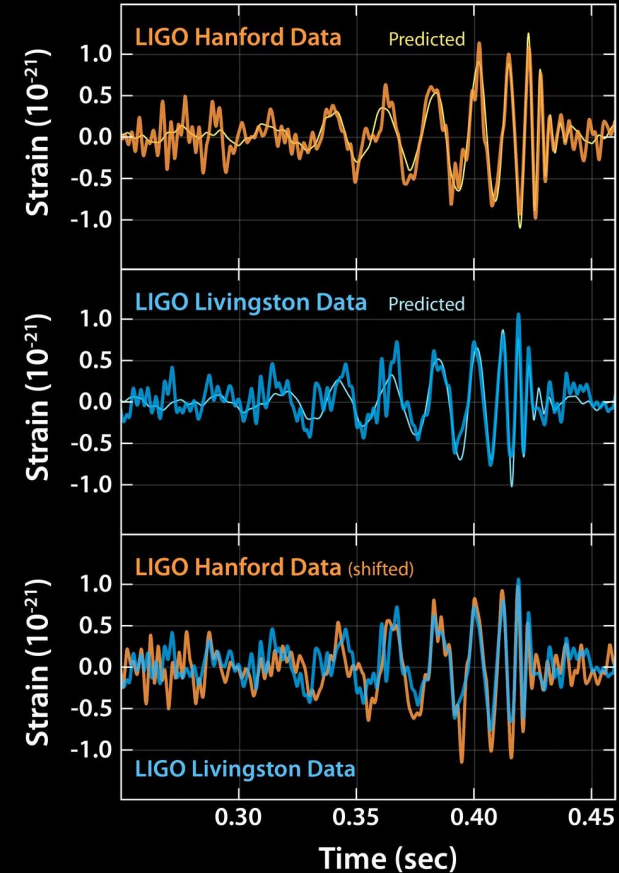
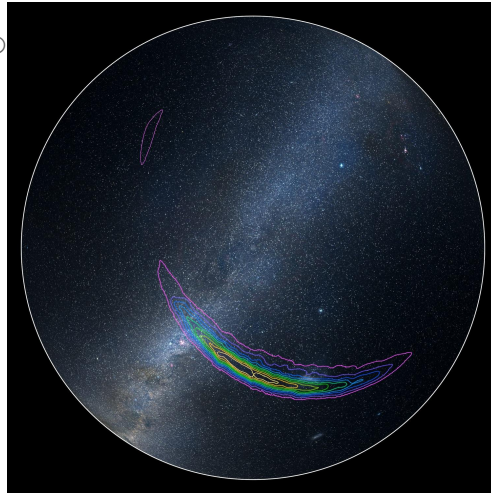




GW150914

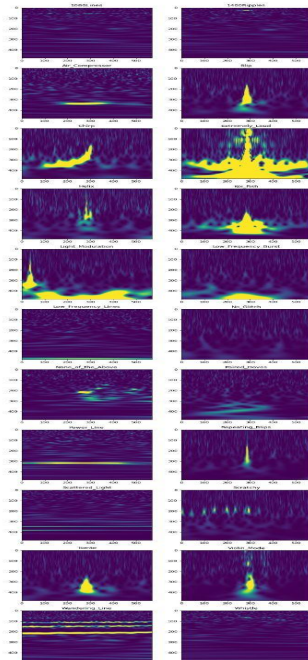
GW150914: la primera
detección

- Fusión de dos agujeros negros.
- Masas: 36 y 31 $M_{\odot}$.
- Energía liberada: 4 $M_{\odot}$.
- Distancia: 1400 millones años-luz.

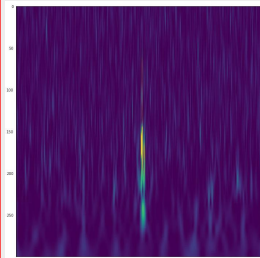
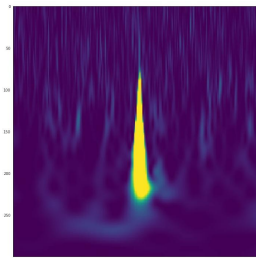


Gravity Spy (Kaggle)

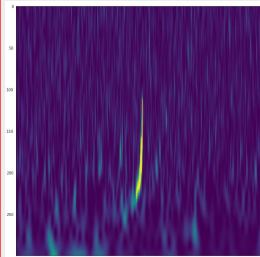
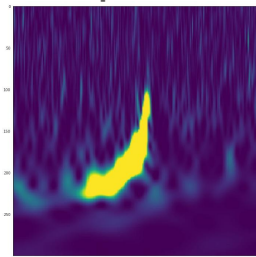
- time-frequency images (Q-transform),
 - 22 labels (chirp + 21 glitches),
 - 31.9k files: train, test, validation;
 - 4 images per event, time window of 0.5, 1, 2, and 4 seconds,
 - strongly unbalanced labels,
 - public data set.
-
- Ideal for testing ideas.
 - Images ideal for Convolutional NN (CNN).
 - Classification per image or per event?



blip



chirp

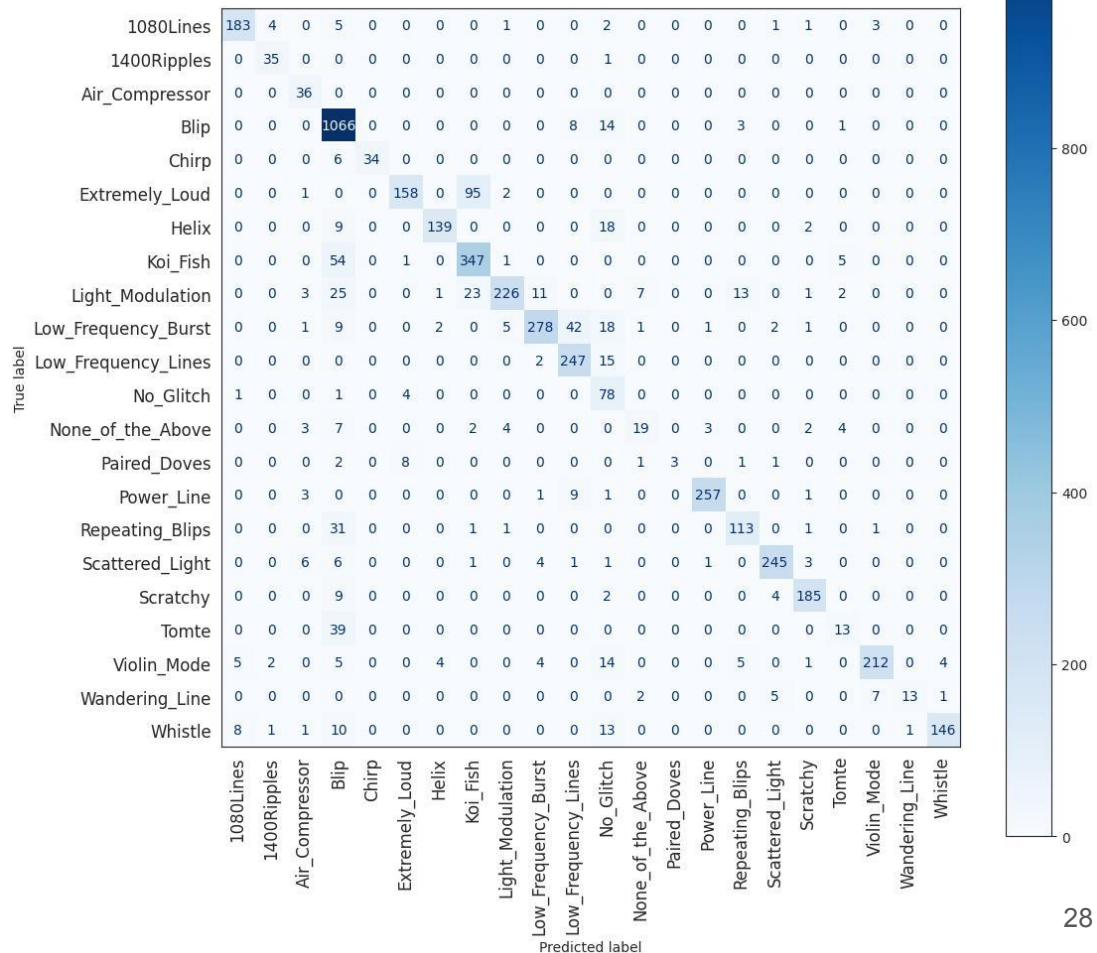


4s

Gravity Spy (Kaggle)

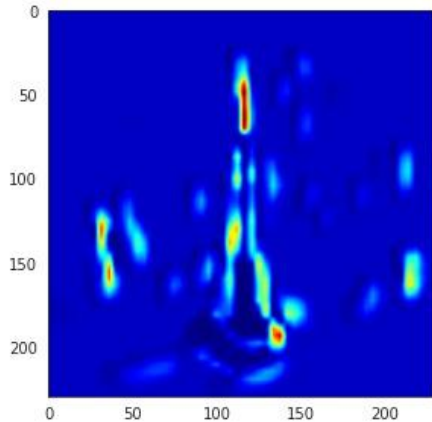
- (2 or 3)X(Conv2D+MaxPooling) + output layer (from 6 to 2 [irreducible] chirp errors).
- Trainable parameters: 1M-400k
- ~190 per epoch
- EarlyStopping patience=3

- Most of the chirp errors go to blip label.
- All the chirp errors are for 4 s time window.

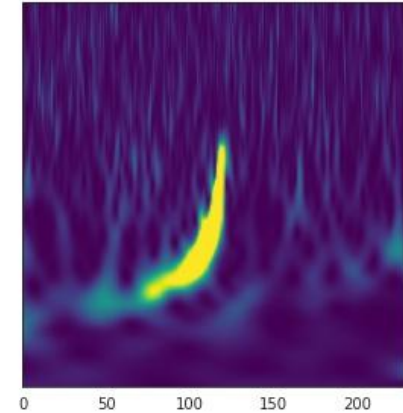
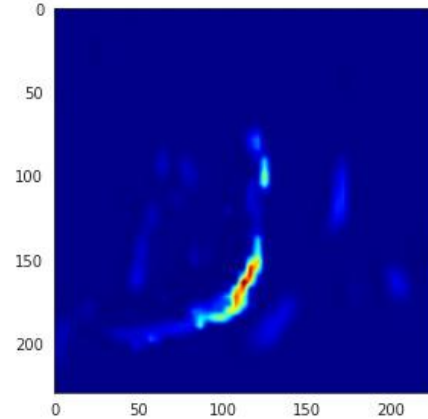
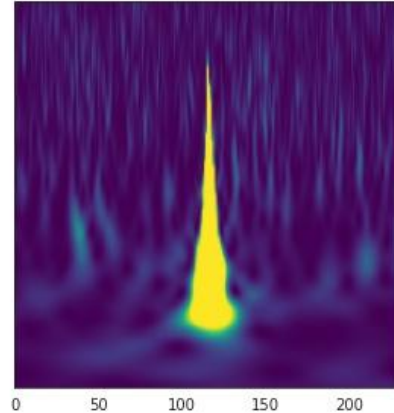


XAI (GradCAM), correctly classified events

Blip

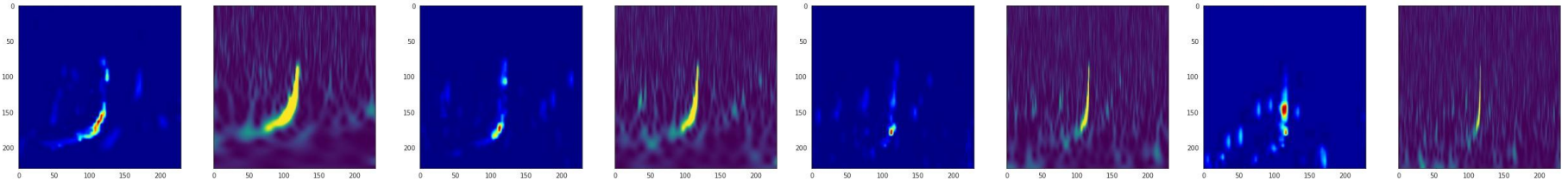


Chirp



Grad-CAM: Visual Explanations from Deep Networks via Gradient-based
Localization <https://doi.org/10.48550/arXiv.1610.02391>

XAI (GradCAM), correctly classified events

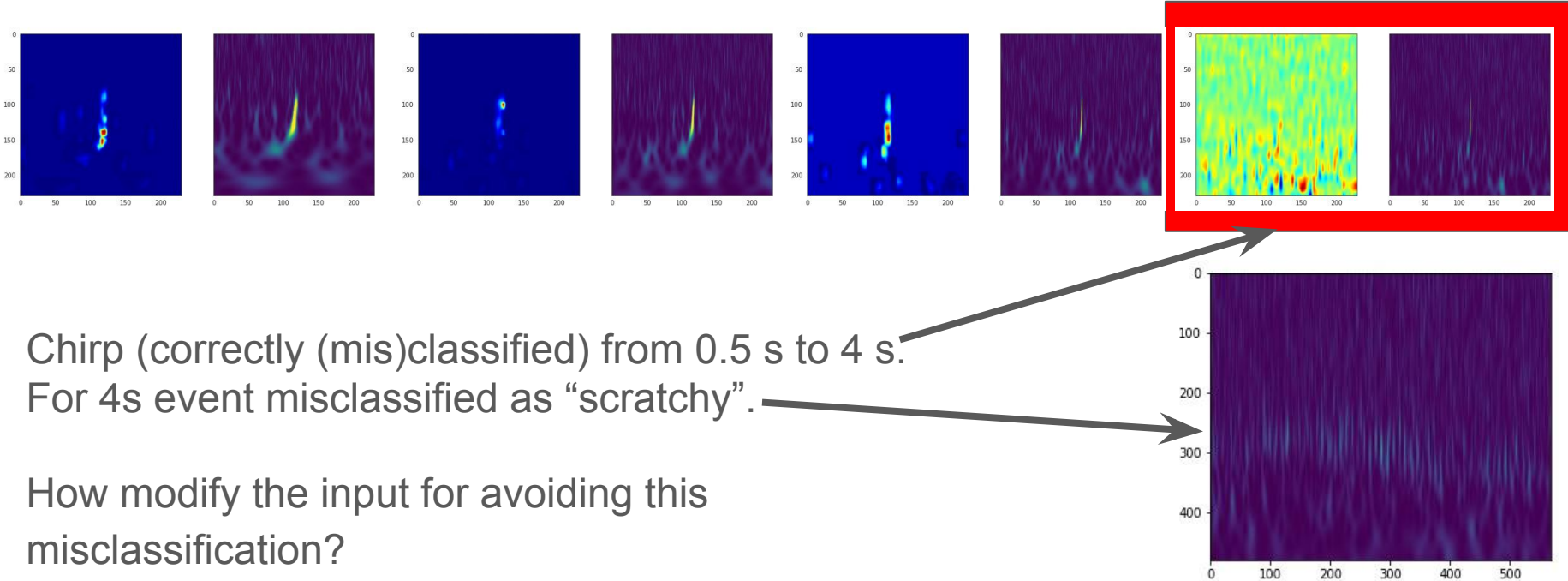


Chirp event (correctly classified) from 0.5 s to 4 s.

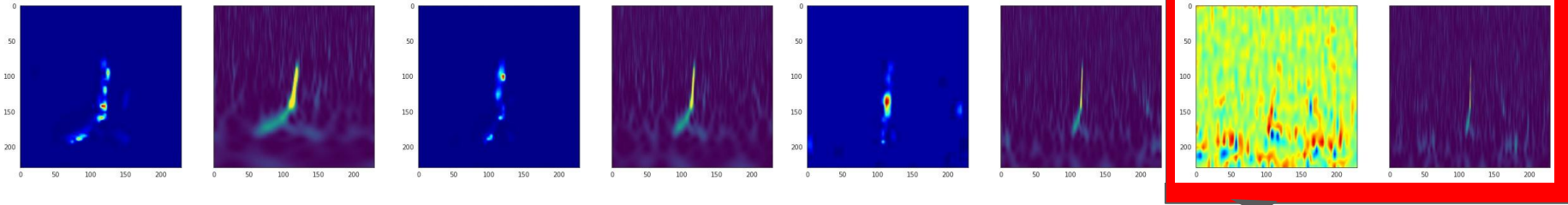
As the window is larger, the image is more stretched vertically.

Horizontal part of the chirp becomes less relevant, and more prone to misclassification.

XAI (GradCAM), incorrectly classified events



XAI (GradCAM), incorrectly classified events

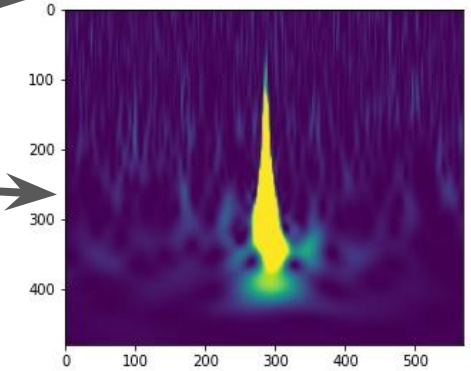


Chirp (correctly (mis)classified) from 0.5 s to 4 s.

For 4s event misclassified as “blip”.

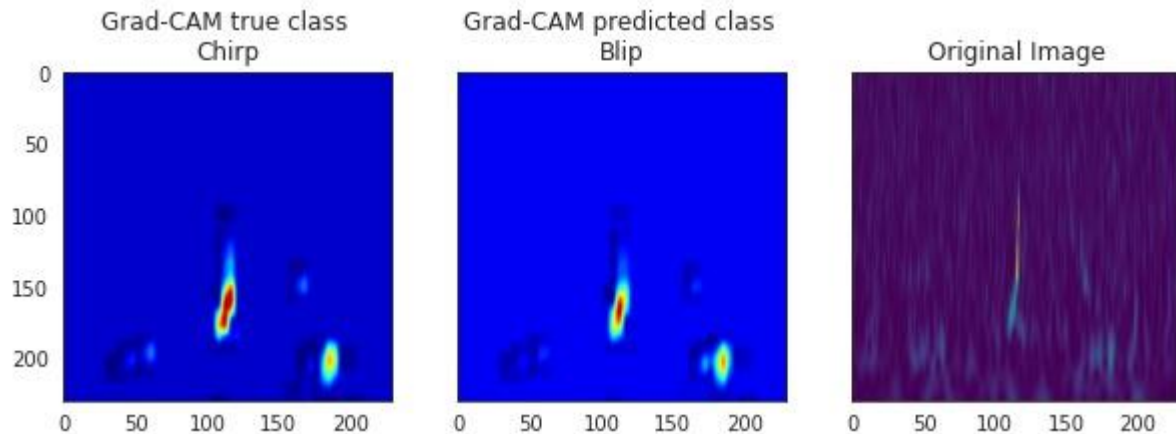
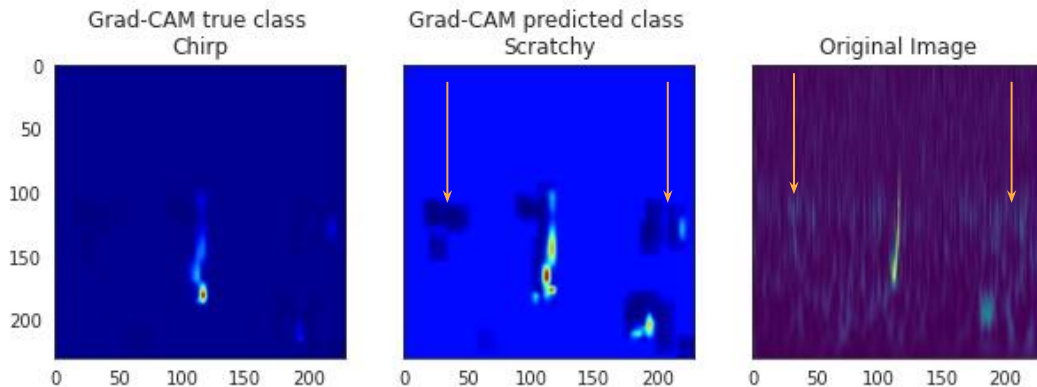
How modify the input for avoiding this misclassification?

New ideas for improving the classification.



XAI (GradCAM), incorrectly classified events

How to modify the input for
remove confusing features
(pixels)?
XAI teaches us how.



XAI (LIME), correctly classified events

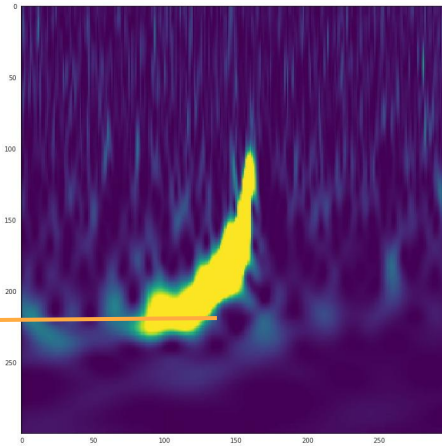
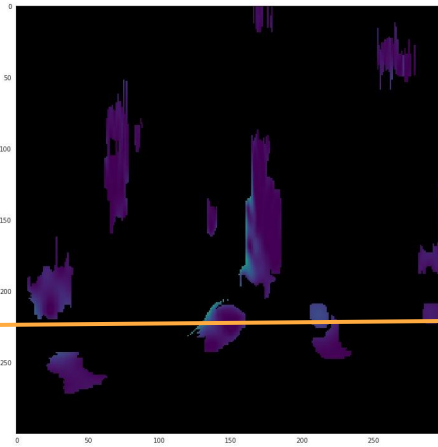
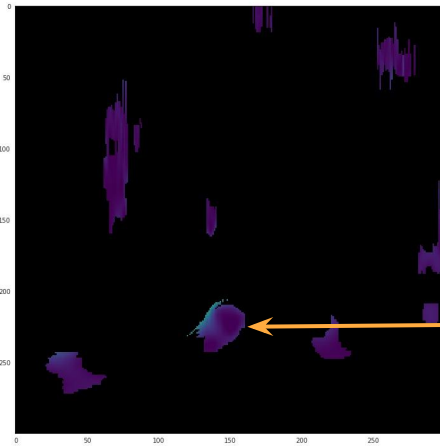
Most relevant patches for correctly classify.

In chirps, ramp-up in frequency is relevant (asymmetric horizontal).

5 parches

10 parches

Chirp

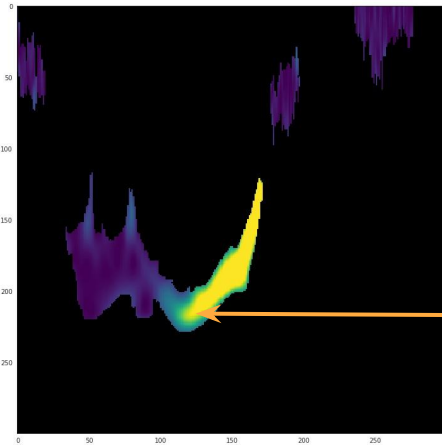


XAI (LIME), correctly classified events

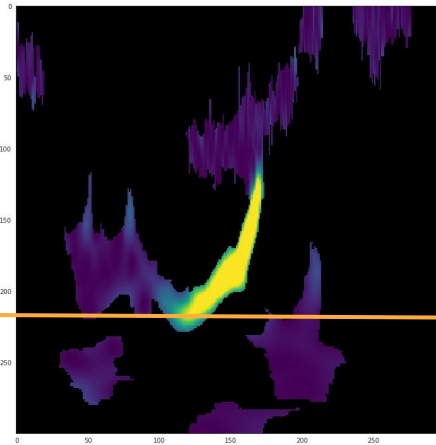
Most relevant patches for correctly classify.

In chirps, ramp-up in frequency is relevant (asymmetric horizontal).

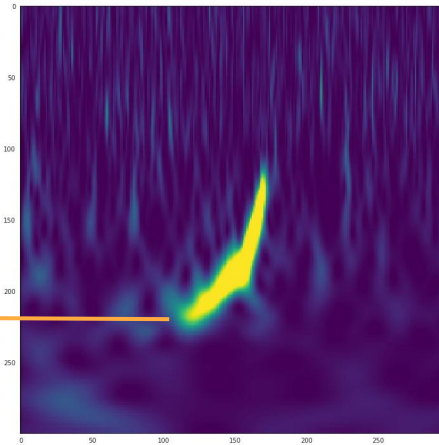
5 parches



10 parches



Chirp

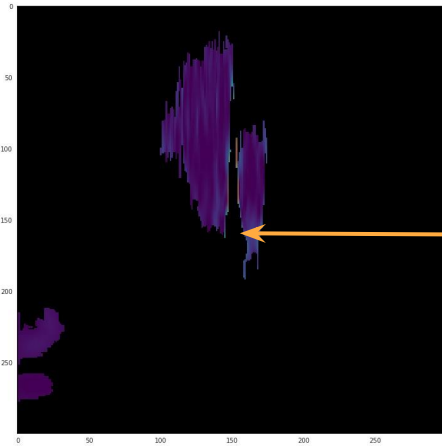


"Why Should I Trust You?": Explaining the Predictions of Any Classifier:
<https://doi.org/10.48550/arXiv.1602.04938>

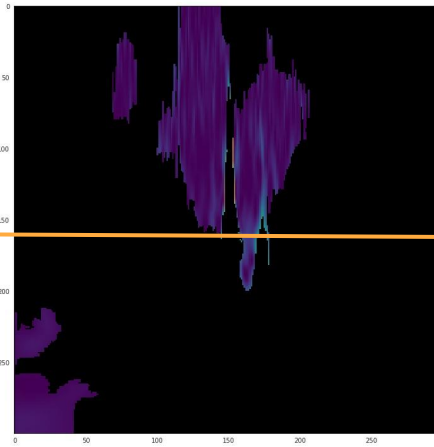
XAI (LIME), correctly classified events

In blips, vertical-lateral to stronger part of the signal is relevant.

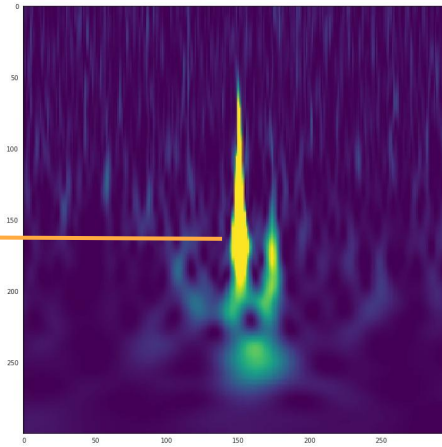
5 parches



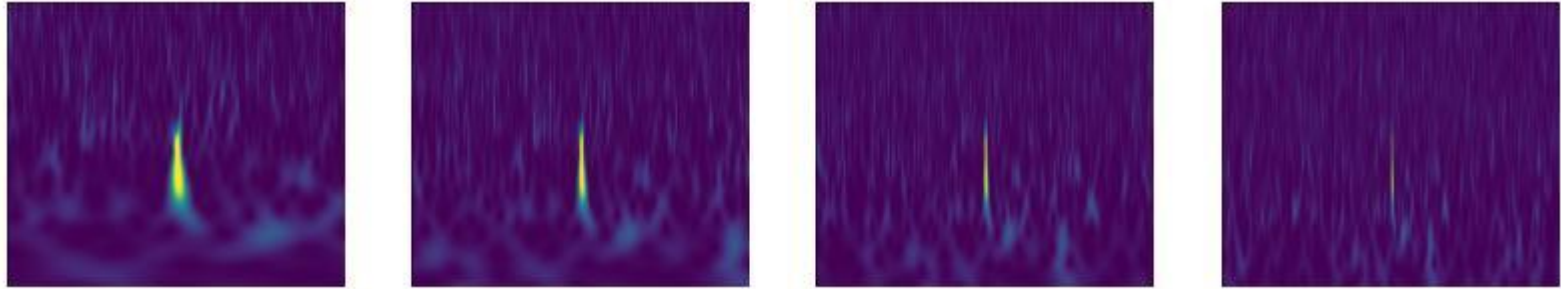
10 parches



Blip



Events as sequences of images (time windows)



Convert 4 images into a sequence (event) -> event classifier

input shape = (4,479,569,3)

```
model.add(layers.Conv3D(8, kernel_size=(1, 3, 3), activation='relu'))
```

instead of:

```
model.add(layers.Conv2D(filters=128, kernel_size=(3,3), activation = 'relu'))
```

Input: multitime tensor data

- No errors on chirps or 1 single error.
- 2D
 - 3 errors
 - 190 s /epoch, ~24 epochs, patience 3
 - 1M-400k trainable parameters.
- 3D
 - 0-2 errors (depends on 2D or 3D SpaAtt)
 - 15 s /epoch, ~4 epochs, patience 3
 - ~ 150k par. Lower carbon footprint
- Spatial Attention layer for interpretability.

Spatial Attention

```
class SpatialAttention(Layer):
```

Spatial attention 3D

```
    .  
    .  
    .  
    self.kernel = self.add_weight(name='kernel',  
                                   shape = (1,1,1,input_shape[-1],1),  
                                   initializer='uniform',  
                                   trainable=True)
```

```
class SpatialAttention(Layer):
```

```
    .  
    .  
    .  
    self.kernel = self.add_weight(name='kernel',  
                                   shape = (1,1,1,input_shape[-1],1),  
                                   initializer='uniform',  
                                   trainable=True)
```

```
    .  
    .  
    .  
    attention = tf.nn.sigmoid(tf.nn.conv3d(x, self.kernel,  
                                             strides=[1,1,1,1,1], padding='SAME'))  
    return x * attention
```

```
inputs = keras.Input(shape=sample_shape)
```

```
# smartly remove this segment if not spatial attention
```

```
SpaAtt = SpatialAttention()(inputs)
```

```
conv1 = layers.Conv3D(8, kernel_size=(1, 3, 3), activation='relu')(SpaAtt)
```

```
maxpool1 = layers.MaxPooling3D(pool_size=(1, 3, 3))(conv1)
```

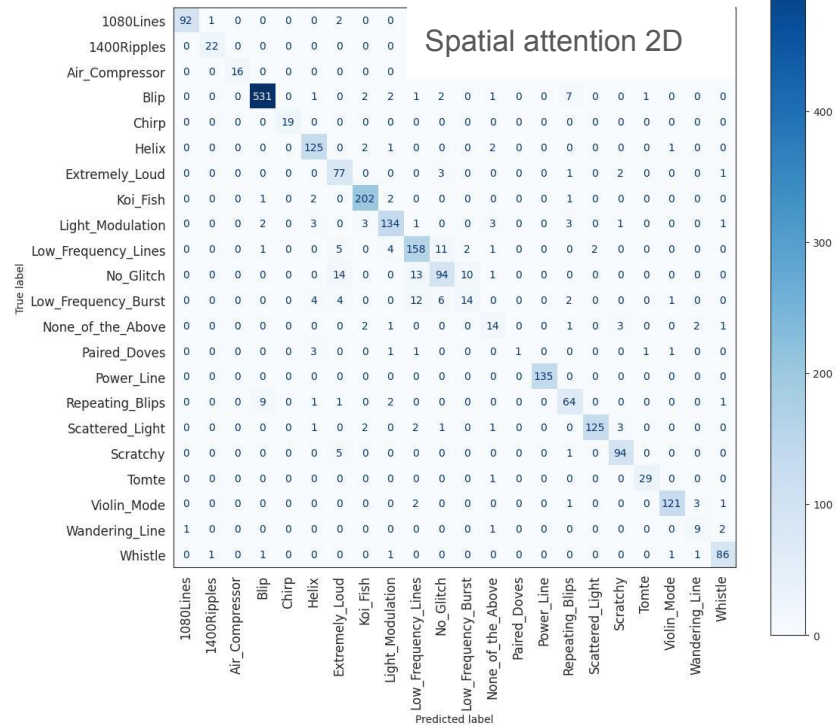
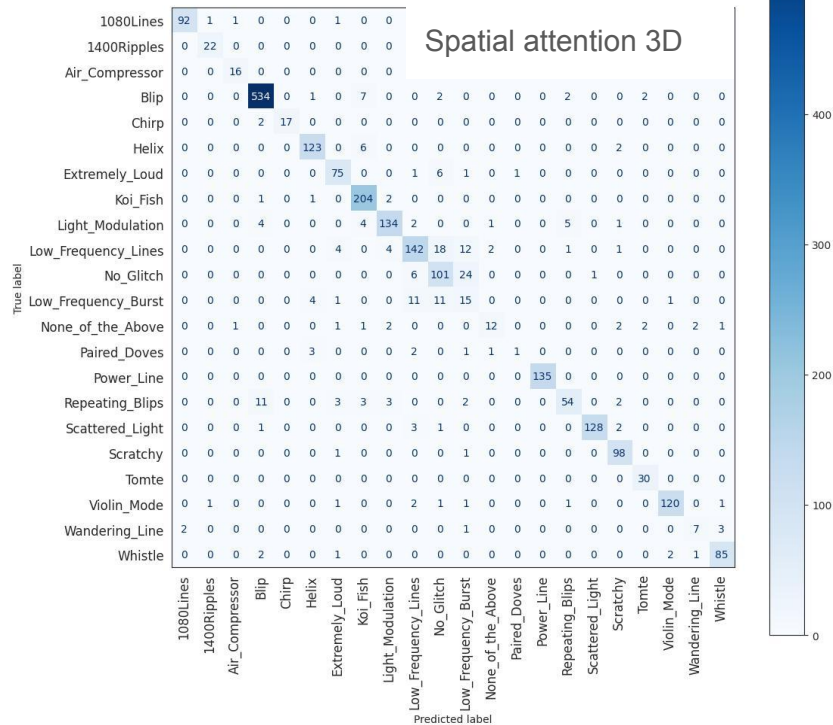
```
self.kernel = self.add_weight(name='kernel',  
                               shape = (1,1,input_shape[-1],1),  
                               initializer='uniform',  
                               trainable=True)
```

Spatial attention 2D

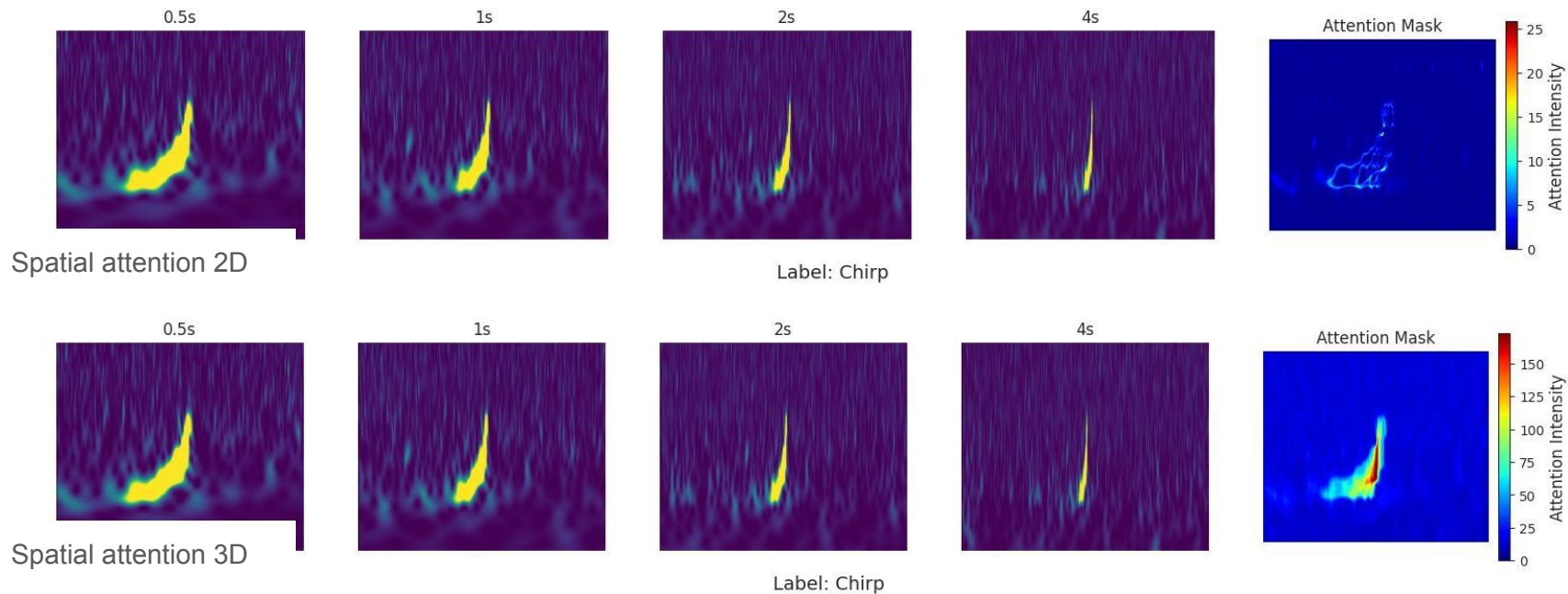
Spatial attention per time layer.

It learns to amplify the pixels of interest, minimizing others.

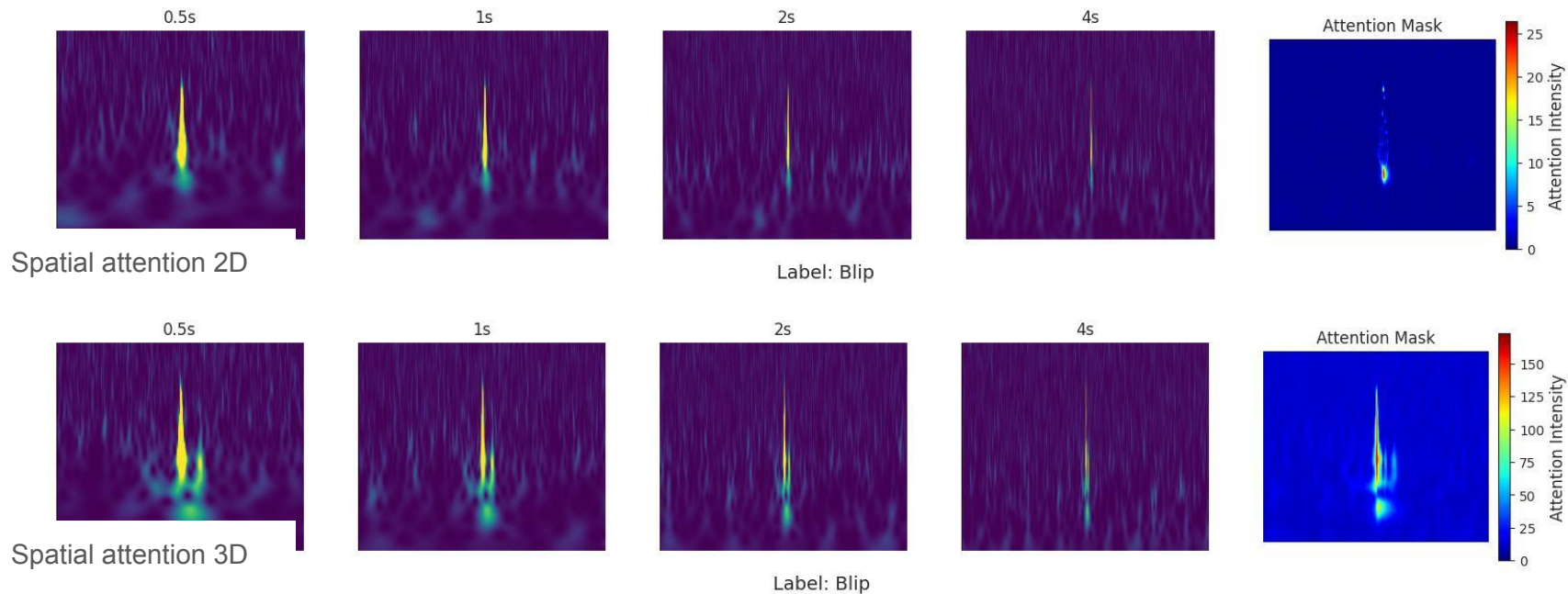
Spatial Attention



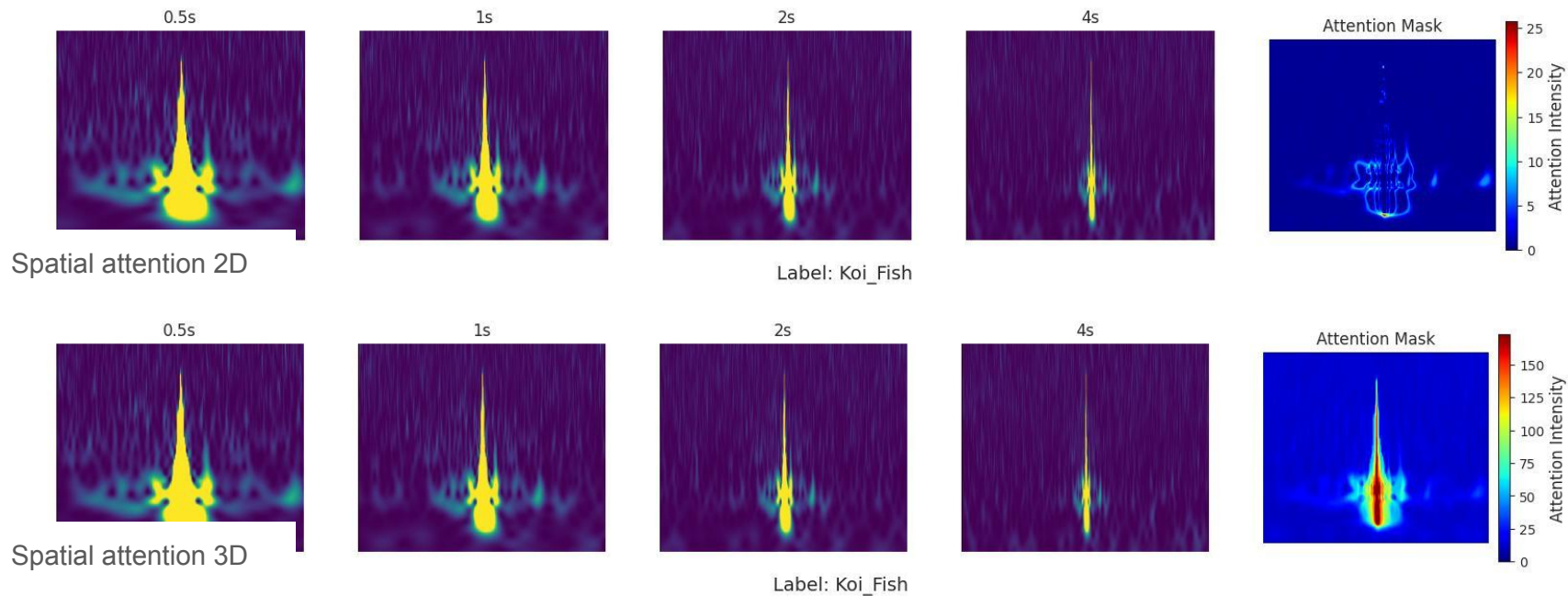
Spatial Attention



Spatial Attention



Spatial Attention



Algoritmos verdes

IA aplicada a IA

CENTROS DE DATOS >

E La IA consumirá en EE UU tanta energía como toda España

La electricidad requerida por los centros de datos se triplicará en tres años, una previsión que podría quedarse corta tras el anuncio de Trump de 500.000 millones en inversiones para desarrollar la inteligencia artificial

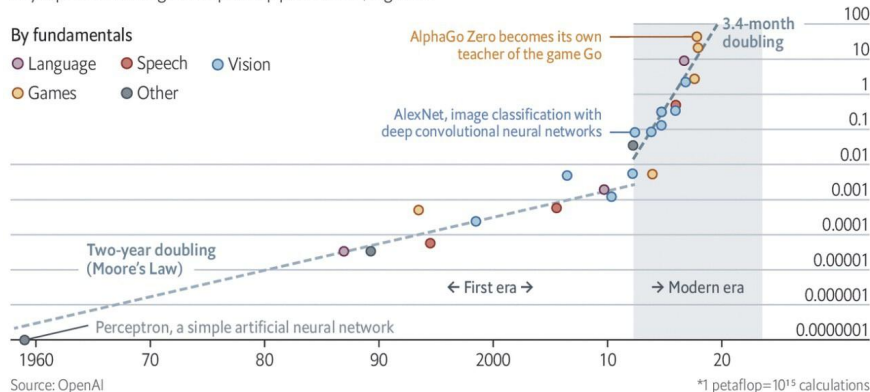
Deep and steep

Computing power used in training AI systems

Days spent calculating at one petaflop per second*, log scale

By fundamentals

- Language
- Speech
- Vision
- Games
- Other



Source: OpenAI

The Economist

Three Mile Island is reopening and selling its power to Microsoft



By Jordan Valinsky, CNN

3 minute read · Updated 12:57 PM EDT, Fri September 20, 2024



New York (CNN) — Three Mile Island, the site of worst nuclear disaster in the United States, is reopening and will exclusively sell the power to Microsoft as the company searches for energy sources to fuel its AI ambitions.

Constellation Energy announced Friday that its Unit 1 reactor, which closed five years ago, is expected to be revived in 2028, dependent on Nuclear Regulatory Commission approval. Microsoft will purchase the carbon-free energy produced from it to power its data centers to support artificial intelligence.

Financial terms of the 20-year agreement, which Constellation called its largest ever, weren't disclosed.

Algoritmos Verdes

La huella de carbono del entrenamiento de ciertas arquitecturas equivale a 5X la vida media de un coche, incluida su manufactura.

Strubell, Ganesh, McCallum: Energy and policy considerations for deep learning in NLP (2019)

El módulo Inception es de uso frecuente en Visión por Computador.

Inception incluye ramas paralelas de filtros convolucionales preconfigurados ¿fijos?

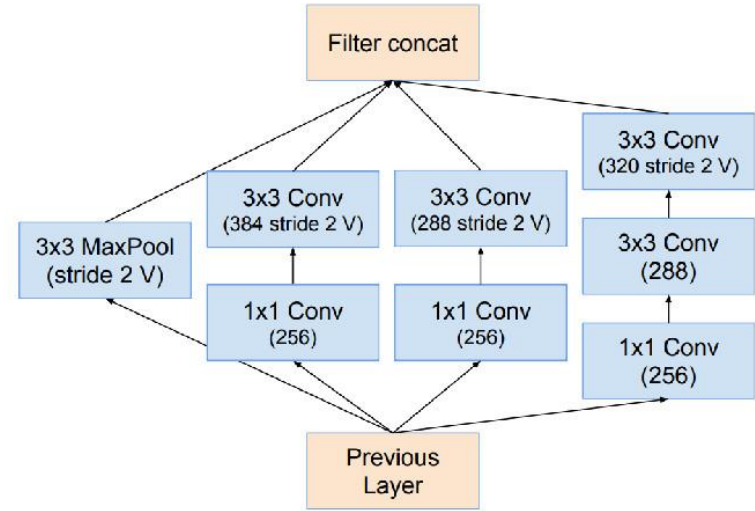
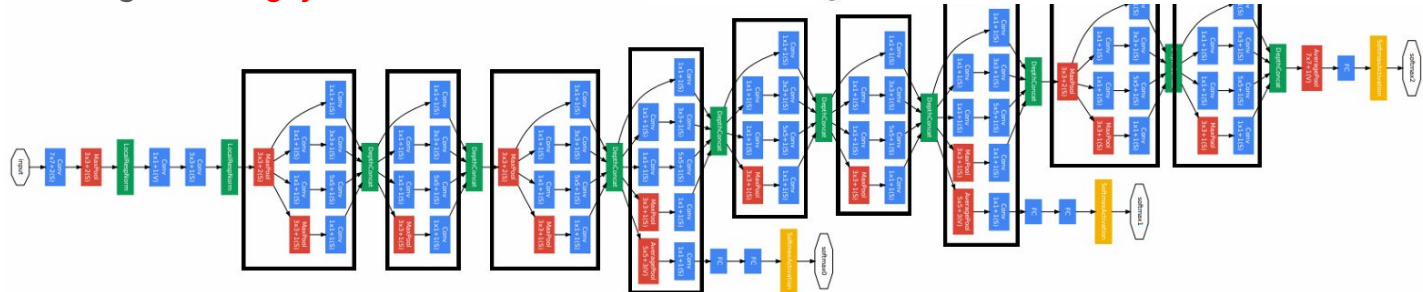


Figure 18. The schema for 17×17 to 8×8 grid-reduction module. Reduction-B module used by the wider Inception-ResNet-v1 network in Figure 15.



Inception

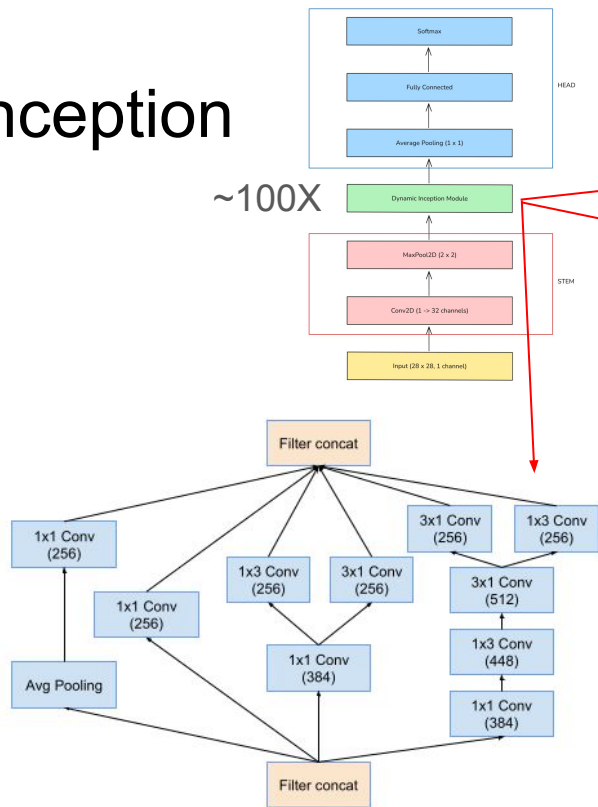


Figure 6. The schema for 8×8 grid modules of the pure Inception-v4 network. This is the Inception-C block of Figure 9

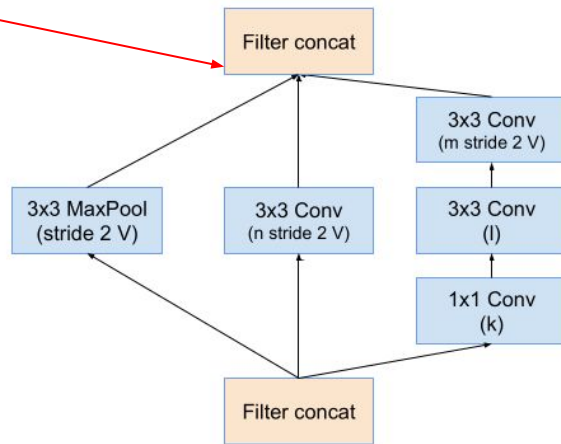


Figure 7. The schema for 35×35 to 17×17 reduction module. Different variants of this blocks (with various number of filters) are used in Figure 9 and 15 in each of the new Inception(-v4, -ResNet-v1, -ResNet-v2) variants presented in this paper. The k , l , m , n numbers represent filter bank sizes which can be looked up in Table 1

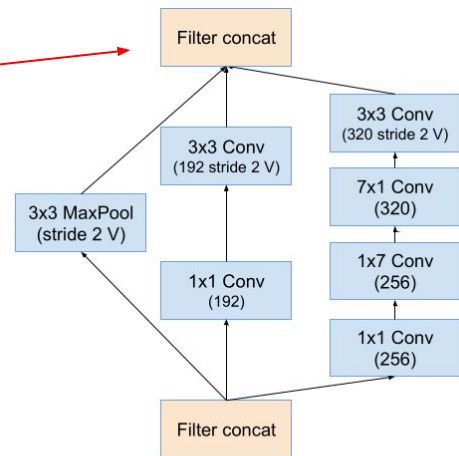


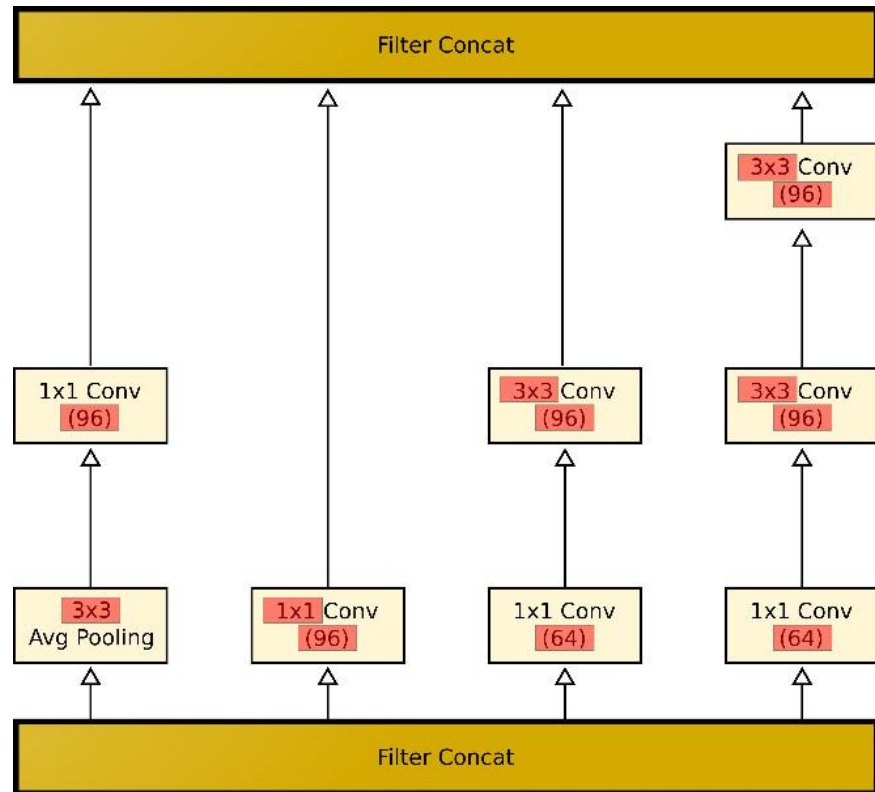
Figure 8. The schema for 17×17 to 8×8 grid-reduction module. This is the reduction module used by the pure Inception-v4 network in Figure 9

Green Algorithms

- Search for new configurations (size and number of filters) of Inception using a combinatorial optimizer: Population based Incremental Learning (PBIL).
- We prohibit configurations with the same filter size in different branches of the Inception module. Why?
- To save time and energy!

```

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1 1 1
2 2 2 2 2 2 2 2 2 2 2 2 2 2
3 3 3 3 3 3 3 3 3 3 3 3 3 3
4 4 4 4 4 4 4 4 4 4 4 4 4 4
5 5 5 5 5 5 5 5 5 5 5 5 5 5
6 6 6 6 6 6 6 6 6 6 6 6 6 6
7 7 7 7 7 7 7 7 7 7 7 7 7 7
8 8 8 8 8 8 8 8 8 8 8 8 8 8
9 9 9 9 9 9 9 9 9 9 9 9 9 9
    
```



PBIL

- PBIL (Population-based incremental learning) es un algoritmo de distribución de poblaciones (EDA).
- PBIL es un algoritmo de optimización. Es similar a un algoritmo genético donde el genotipo de la población (vector de probabilidad) evoluciona con los individuos de la población.
- PBIL es como sigue:
 1. Una población es generada con un vector de probabilidad, **P**.
 2. El fitness de cada individuo de la población es evaluado y los individuos ordenados por él.
 3. Se actualiza el genotipo de la población (vector probabilidad) tomando como base los
 4. mejores individuos de la población.
 5. Se establece un operador de mutación para el vector probabilidad.
 6. Repetir pasos de 1 a 4.

PBIL

- Se utiliza un vector de probabilidades **P** para generar las nuevas soluciones en cada iteración.
- La distribución de probabilidad almacena la información acerca de la frecuencia de aparición de cada alelo (carácter discreto).
- Para evitar una convergencia prematura, se aplica un operador de mutación sobre el vector de probabilidades.

Codificación Gray

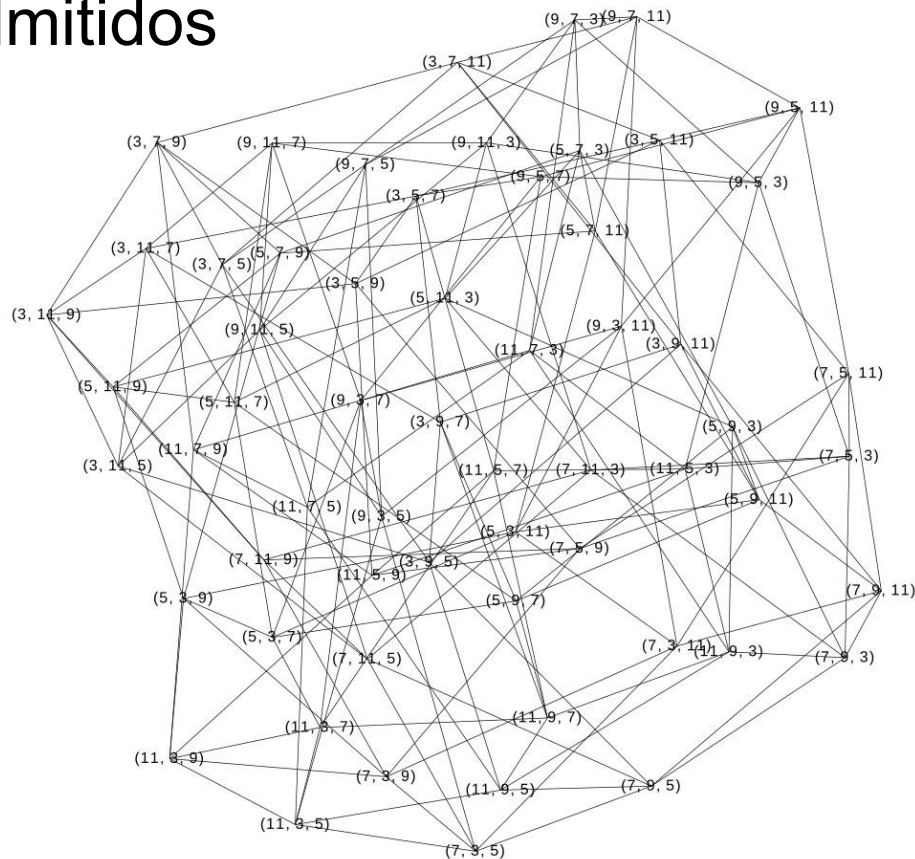
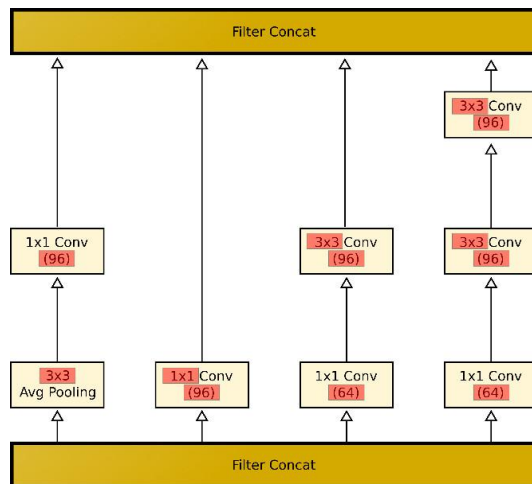
Los valores posibles del número de filtros y sus tamaños codificados con Codificación Gray para evitar Hamming Cliff:

1. En binario: 3 (0011) y 4 (0100), distancia Hamming de 3.
2. Empeora a medida que los números son mayores: 8 (0111) y 9 (1000), distancia Hamming de 4.

Decimal	Binario	Gray
0	0000	0000
1	0001	0001
2	0010	0011
3	0011	0010
4	0100	0110
5	0101	0111
6	0110	0101
7	0111	0100
8	1000	1100
9	1001	1101
10	1010	1111

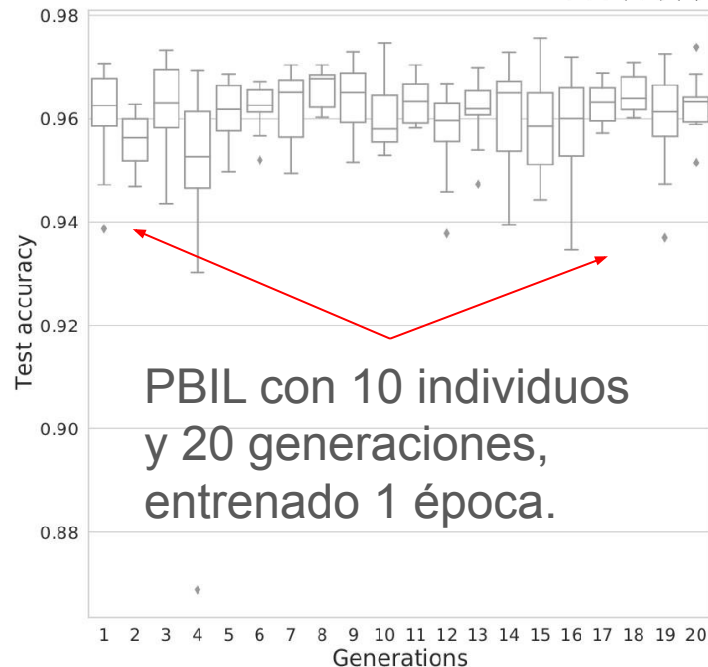
Grafo de tamaño de filtros admitidos

Grafo representando todas las configuraciones de los filtros admitidas a distancia Hamming 1. PBIL se mueve a lo largo del camino Hamiltoniano.

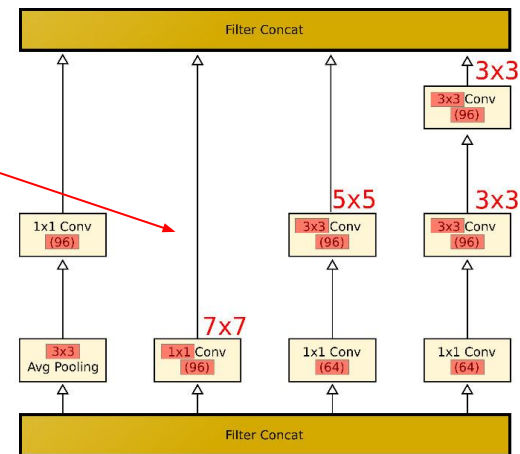


[illegible]

Resultado: MNIST



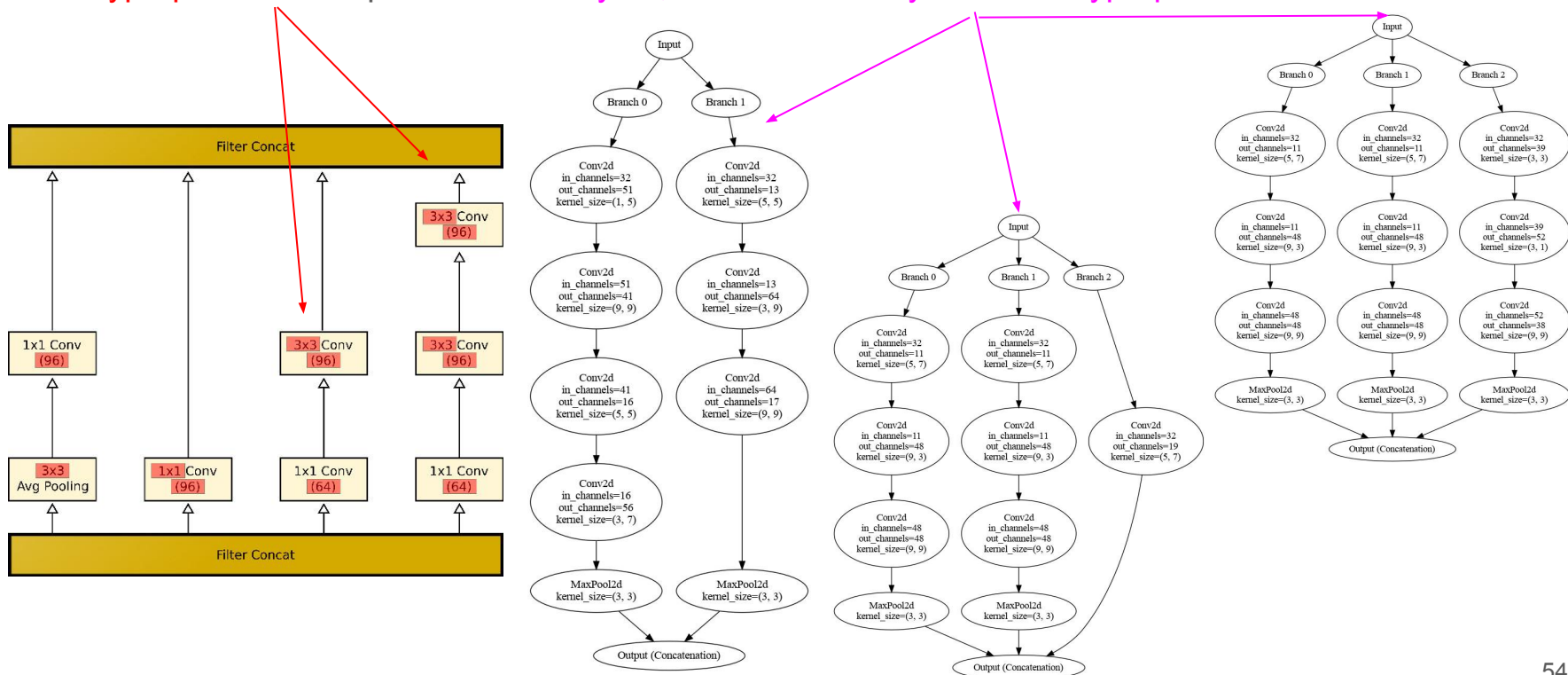
Mejor individuo
entrenado con early
stopping (5 épocas).



Mejor individuo para problema
MNIST (0.9922)
O(-1) # parámetros (0.9987)
O(-2) # épocas (0.9984)

Green Algorithms, more flexibility

From **hyperparameters** optimization to **layers, their connectivity and their hyperparameters**.



Green Algorithms, more flexibility

Optimization to **layers, their connectivity and their hyperparameters.**

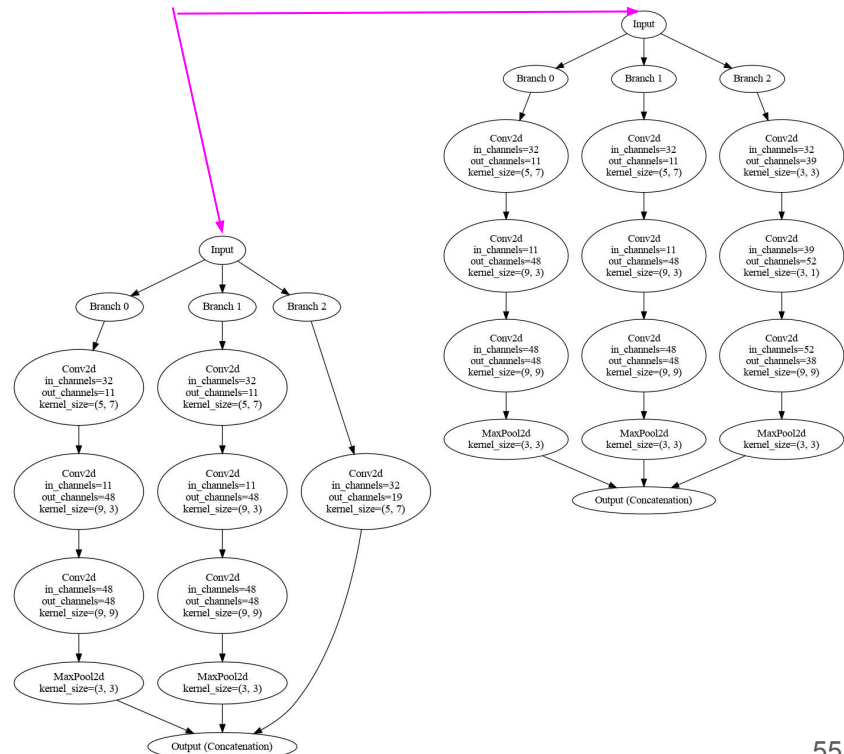
When are these kinds of optimized architectures valuable?

Optimized architectures become essential in cases where **progressive retraining** is mandatory due to the continuous incorporation of new data into the training set.

In such scenarios, the newly added data can improve the problem being addressed. For instance, it can **help balance previously imbalanced datasets**, especially when the new data corresponds to previously underrepresented labels.

This is also relevant when **new classes need to be introduced** into the problem. Additionally, and equally important, a larger number of samples may become available compared to the past.

In these cases, periodic retraining of neural networks is essential. Therefore, designing **the most lightweight architecture that maintains performance is highly valuable for rapid reprocessing**, while also helping to limit the carbon footprint of the activity.



Green Algorithms, more flexibility

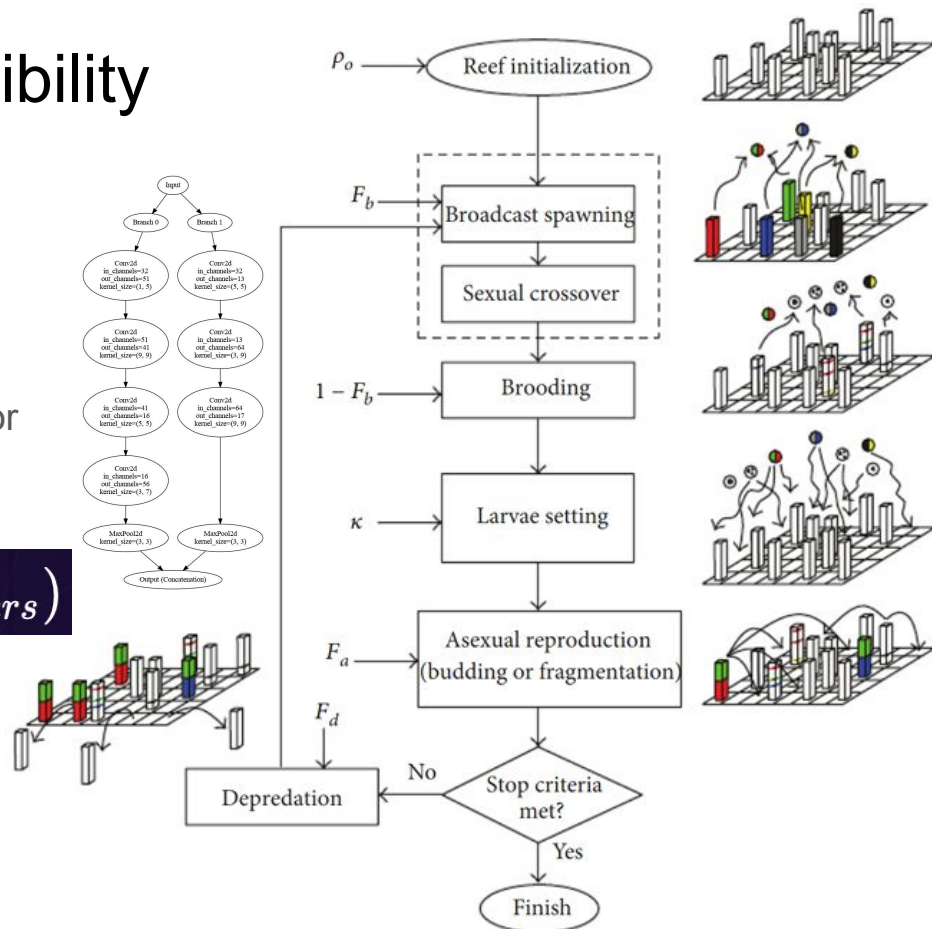


Coral Reef Optimizer

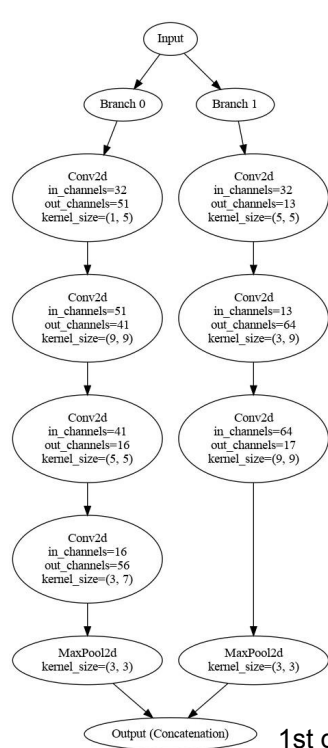
Based on the competition among species for space on coral reefs.

$$F = Accuracy - \alpha \times \log(N_{parameters})$$

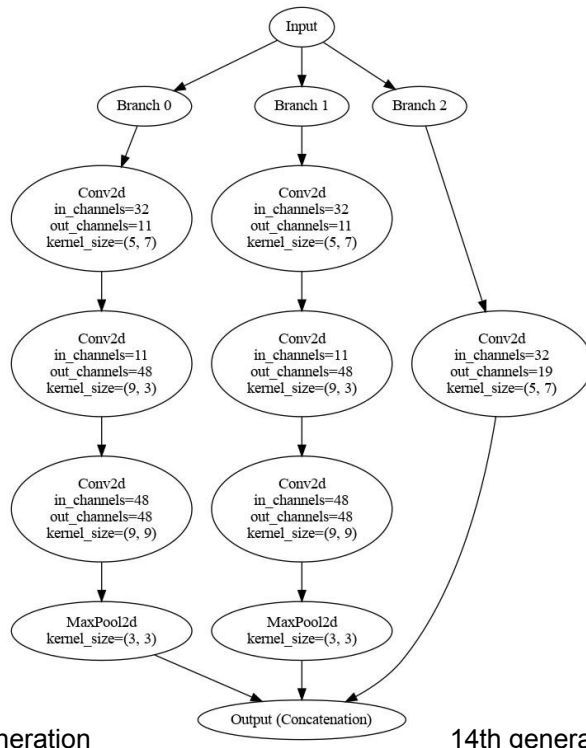
To promote smaller, resource-efficient architectures, we introduce a custom evaluation metric that balances accuracy and model complexity by penalizing excessive parameters.



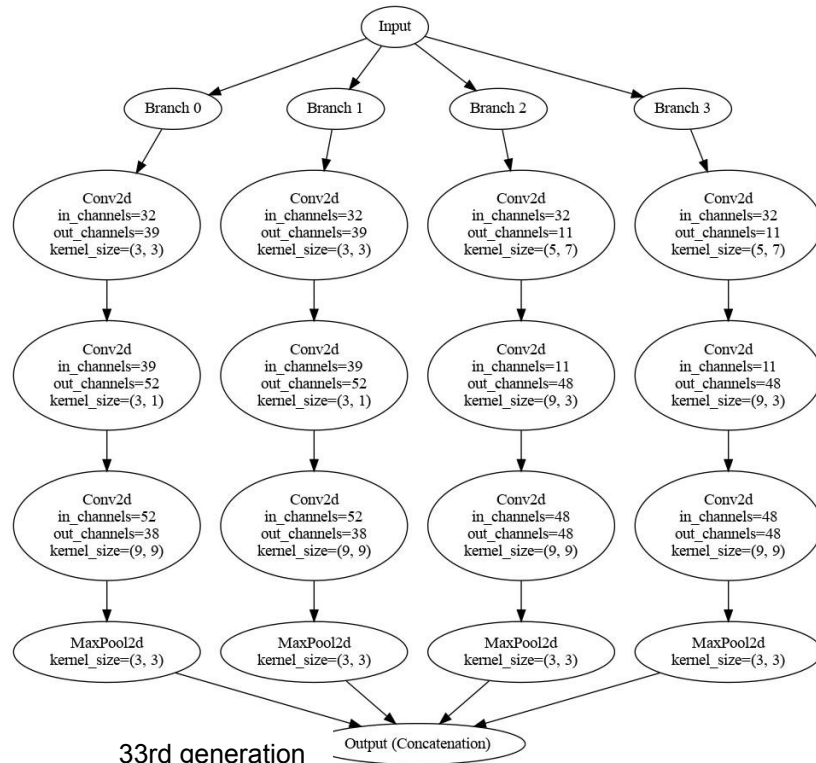
Green Algorithms, more flexibility



1st generation



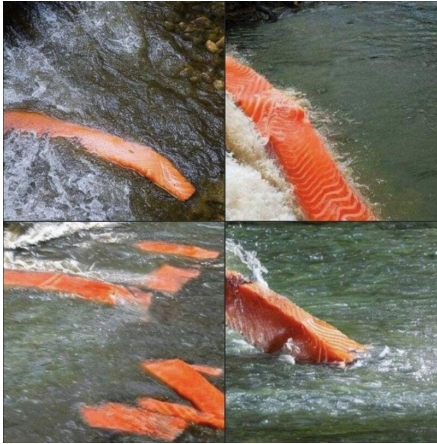
14th generation



33rd generation

Accuracy 98.92 with 805.370 parameters.

Inteligencia Artificial Generativa



Generative Artificial Intelligence, promises



The promise

Collapse Mode



The reality

Human supervision required is infeasible for large sets of new instances.

Artificial intelligence was asked to make a picture of Mother Teresa fighting against poverty.



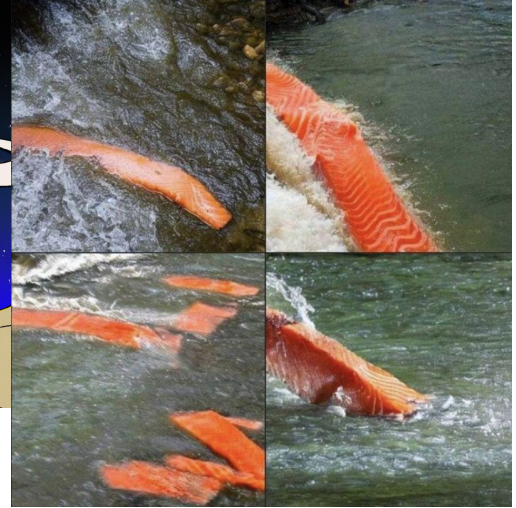
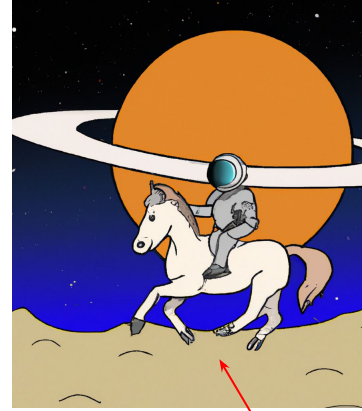
Create a picture of an empty room with no elephant. Absolutely no elephant anywhere in the room

ChatGPT



Here's another depiction of an empty room, designed with a modern and minimalist approach, and importantly, without any elephants.

¿Cómo reconocer ejemplos generados con IA?



Impacto en toda la sociedad: periodismo, política, judicial...

Dependencia de los ejemplos de entrenamiento.

The problem

Generative Artificial Intelligence has revolutionized various sectors by demonstrating its prowess in creating realistic content based on learned patterns from existing examples.

few

However, the new contents (photos, songs, videos) **still need of human verification** for evaluating their realism.

Human-based verification may be impractical for large volume of new instances.

In scientific disciplines, we want to use when not model is available (for instance in oncology), when the examples of interest are only a tiny part of the bulk of simulations (particle physics), or when simulations are expensive (fluid simulation).

many

Newly generated instances need non-human-based supervision mechanisms for evaluating the diversity of the generated instances and metrics for measuring the fitting of generated instances to the true instances or to models based on the true instances are mandatory.

Need an non-human-based supervision mechanism.

Data & Distinguishable features

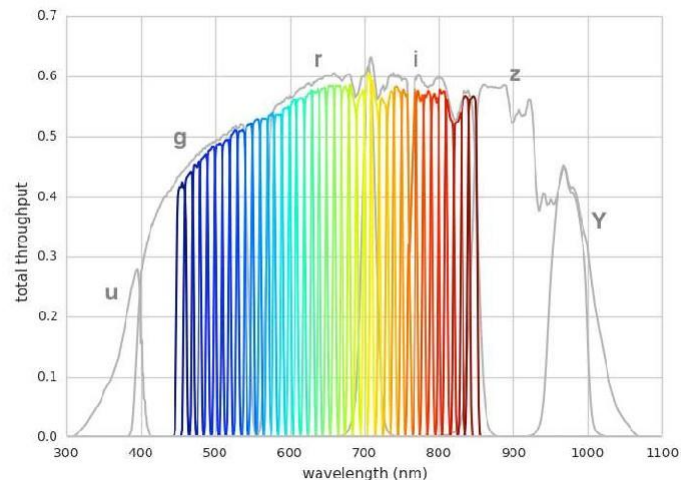
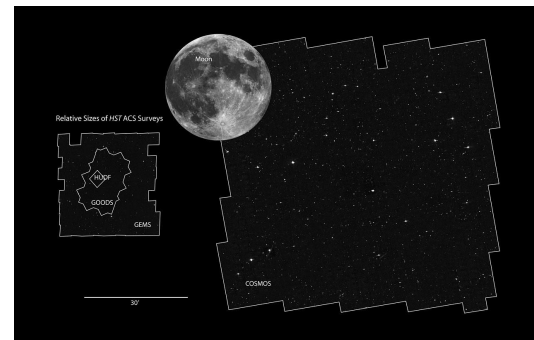
COSMOS Field:

- Area a square of 2 deg^2
- #Galaxies: 40672
- Multi-wavelength:
 - 10 Broad bands:
 - u from the Canada-France Hawaii Telescope
 - B, V, r, i, z from Suprime-Cam/Subaru
 - Y, J, Ks from VIRCAM/VISTA
- Labels of type of galaxies to train: A. Alarcón et al 2021.
- 3 categories: 0 red (7089, early), 1 green(6032) and 2 blue (27551, late).

Espirales



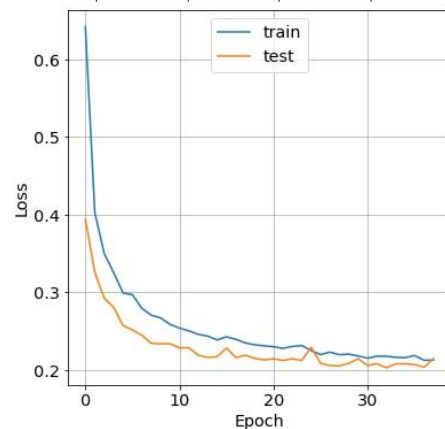
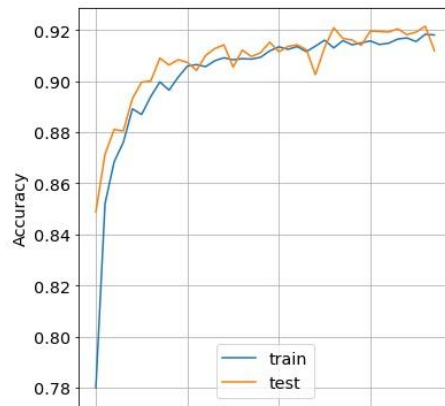
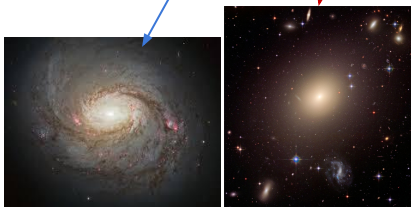
Elípticas



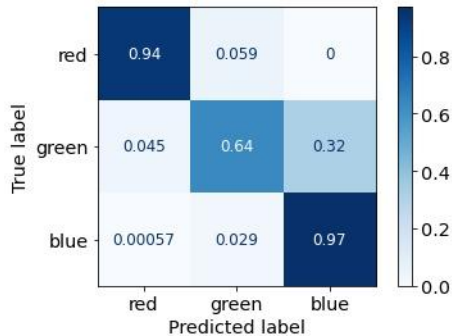
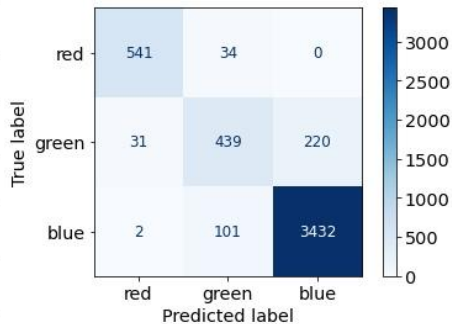
Data & Distinguishable features

COSMOS Field:

- Area a square of 2 deg²
- #Galaxies: 40672
- Multi-wavelength:
 - 10 Broad bands:
 - u from the Canada-France Hawaii Telescope
 - B, V, r, i, z from Suprime-Cam/Subaru
 - Y, J, Ks from VIRCAM/VISTA
- Labels of type of galaxies to train: A. Alarcón et al 2021.
- 3 categories: 0 red (7089, early), 1 green(6032) and 2 blue (27551, late).



shadow MLP with early stopping



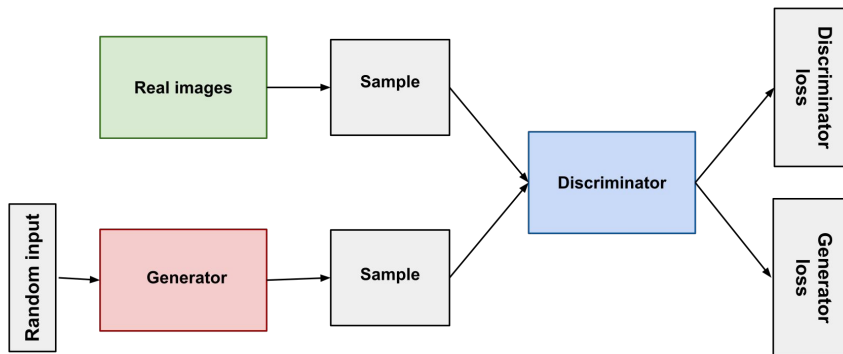
The work

The scarcity-imbalance of certain astronomical objects underscores the importance of enlarged datasets with Generative Artificial Intelligence.

cGAN can generate targeted instances based on limited examples, thus we can build balanced classifiers.

cGAN (MLP-based) with 250 epochs with ~40k galaxy samples.

It takes 100 s/epoch in a GPU. **Then ...**



GP model is trained with a subset (250) of true red galaxies.

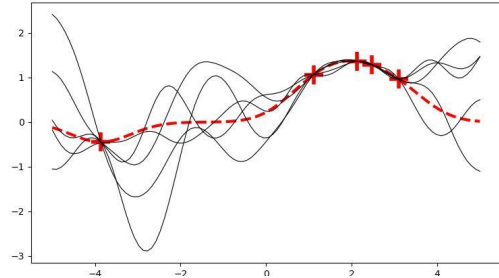
GP model implements *Rational Quadratic* and *White Noise* kernels.

It takes around 325 s.

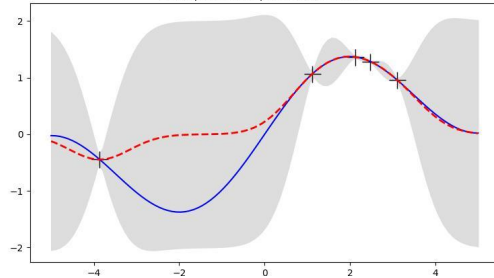
The deviation between the generated instances and the GP model is assessed.

Procesos Gaussianos, intuición

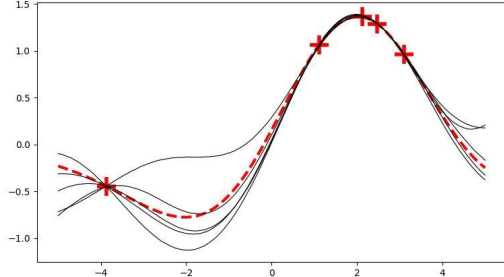
5 samples from the GP posterior, mean prediction function and observation points



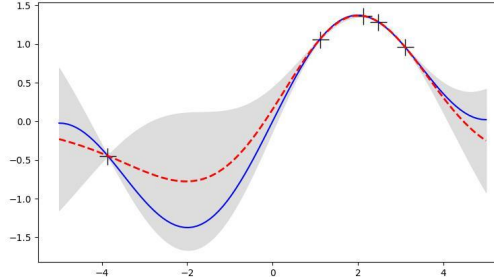
Mean predictions plus 2 st.deviation



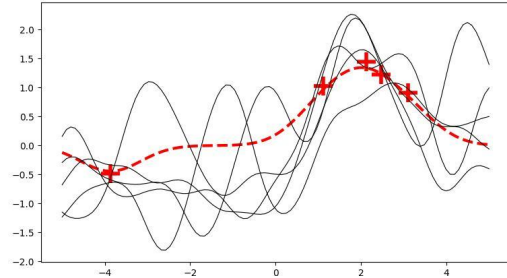
5 samples from the GP posterior, mean prediction function and observation points



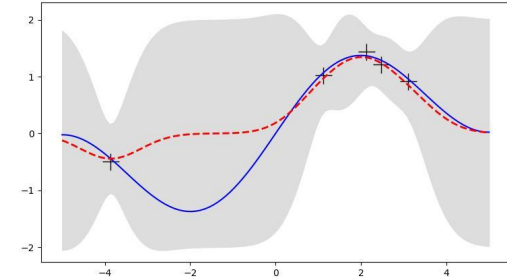
Mean predictions plus 2 st.deviation



5 samples from the GP posterior, mean prediction function and observation points

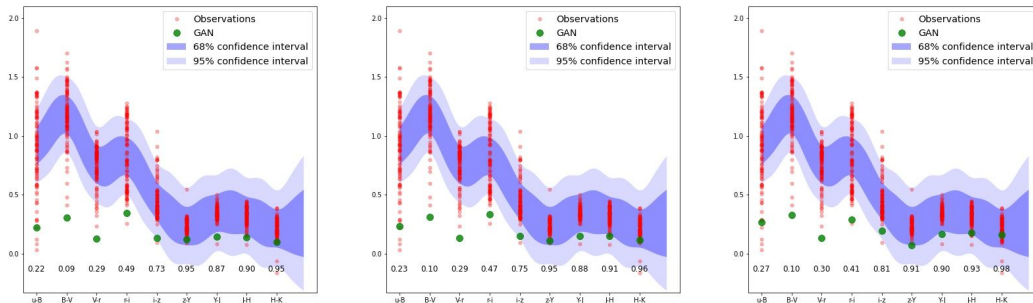


Mean predictions plus 2 st.deviation

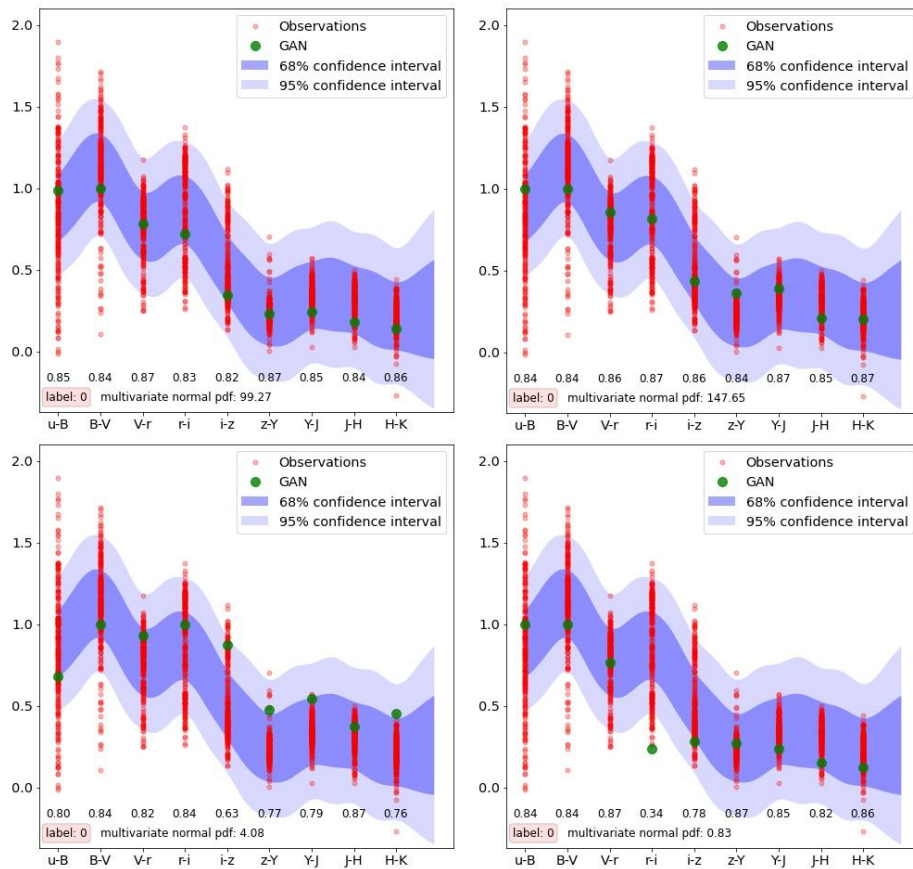


Collapse mode in GAN

- Collapse mode can be caused by lack of variety in the training data, or inadequate network architecture.
- Collapse mode negatively impacts the quality and diversity of the generated instances.
- Variety of generated instance must be evaluated.
- With hundred or thousand of newly generated galaxies impractical for human-based verification.



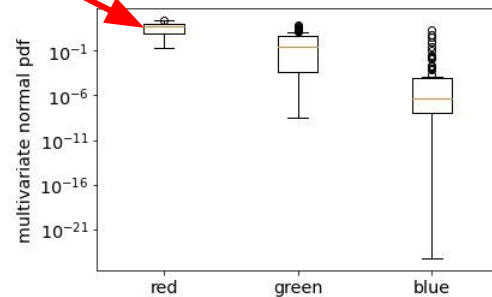
Almost equal result of newly generated instances of GAN.

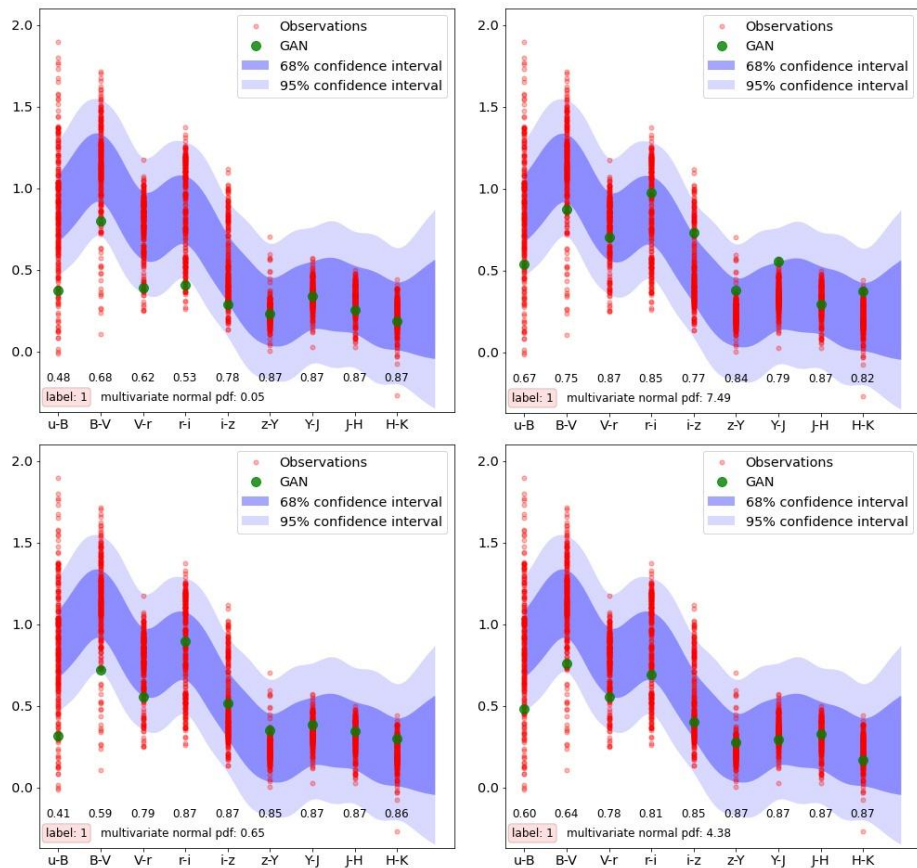


Class 0, red galaxies

Comparison between instances of red galaxies (class 0) generated using the cGAN architecture and the GP model based on true red (class 0) galaxies.

Generated instances well aligned with the model.

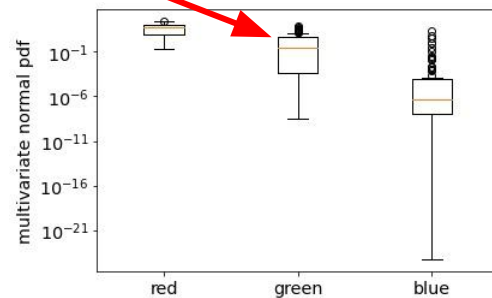


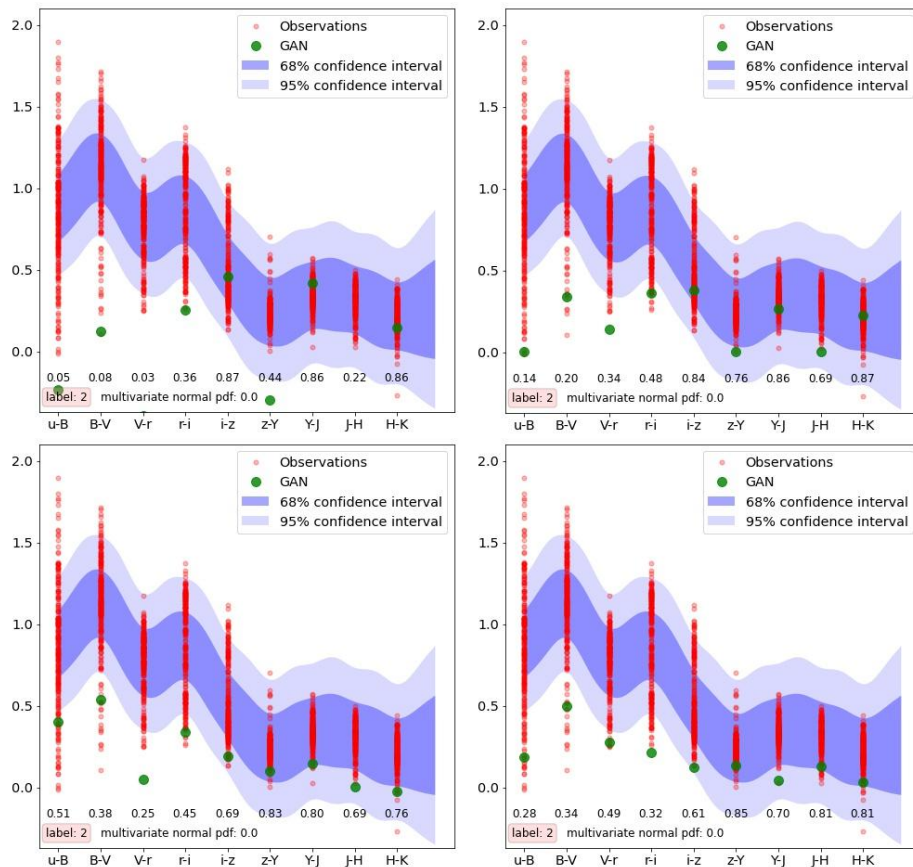


Class 1, green galaxies

Comparison between instances of green galaxies (class 1) generated using the cGAN architecture and the GP model based on true red (class 0) galaxies.

Generated instances less aligned with the model.

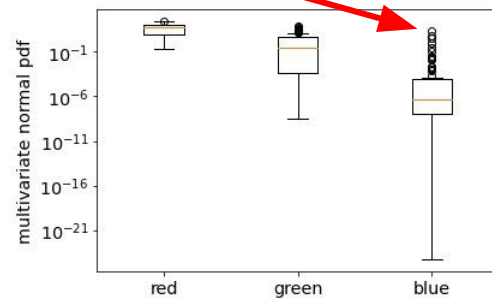




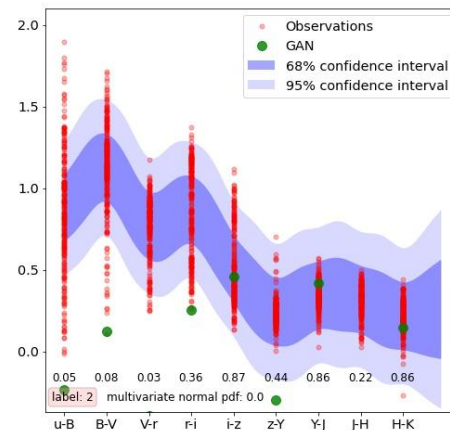
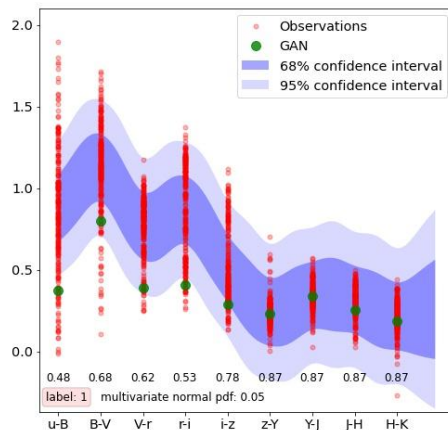
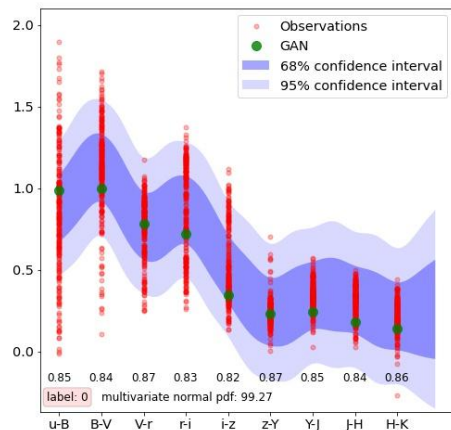
Class 2, blue galaxies

Comparison between instances of blue galaxies (class 2) generated using the cGAN architecture and the GP model based on true red (class 0) galaxies.

Generated instances not aligned with the model.



Visual comparison



Divulgación



Divulgación



Algoritmos Evolutivos



Peso
3

Peso
5

Peso
7

Peso
11

Peso
13

Peso
17

Peso
19

Peso
23

Peso
29

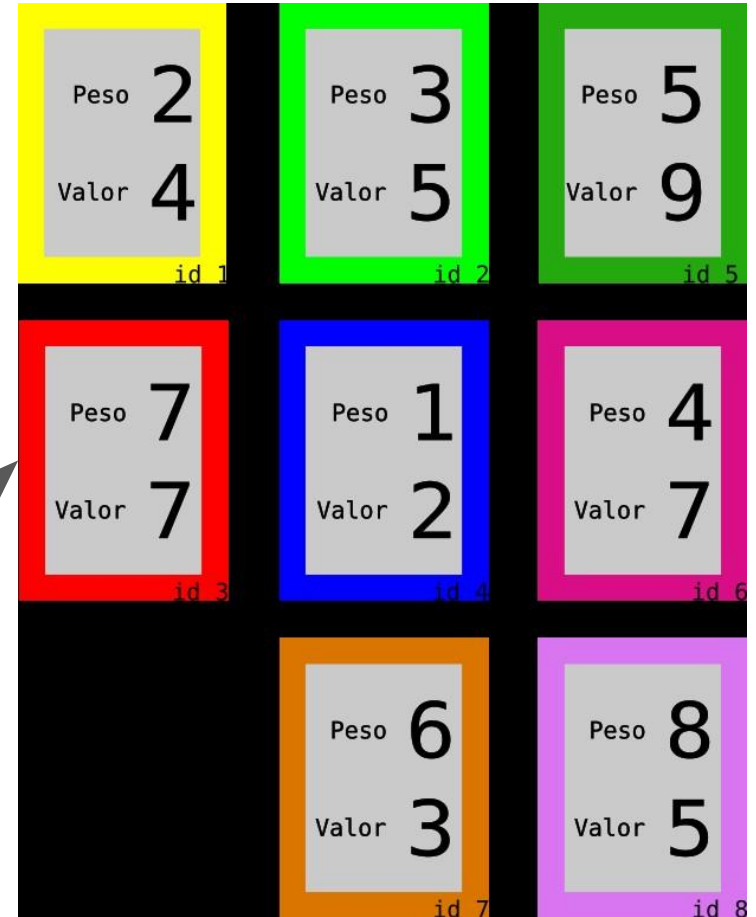
Peso
31

Repartir los objetos
entre dos cohetes de
forma que porten la
misma carga.

Algoritmos Evolutivos

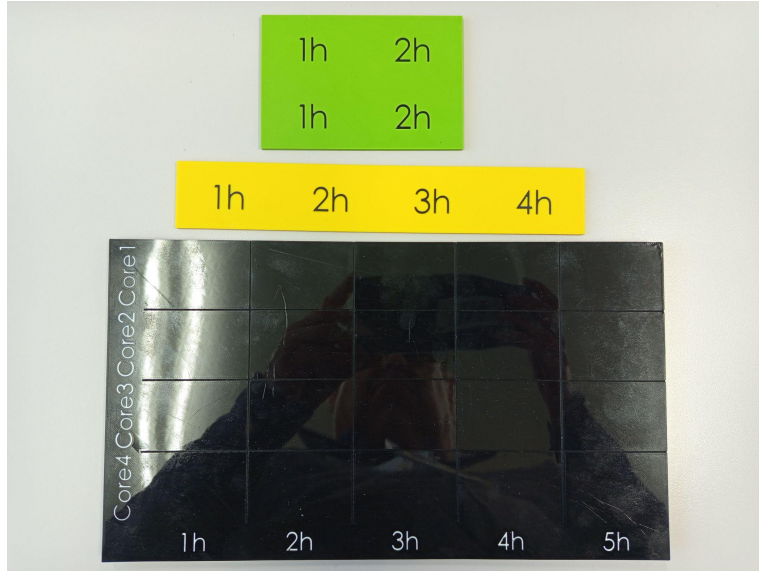
- Los algoritmos evolutivos son ampliamente utilizados en ciencia y en la industria, por ejemplo en logística de mercancías, flotas de aviones, etc.

Problema de la mochila:
maximizar el valor de carga
para un peso máximo: 15.



Peso 2 Valor 4 id 1	Peso 3 Valor 5 id 2	Peso 5 Valor 9 id 5
Peso 7 Valor 7 id 3	Peso 1 Valor 2 id 4	Peso 4 Valor 7 id 6
	Peso 6 Valor 3 id 7	Peso 8 Valor 5 id 8

Job Scheduling



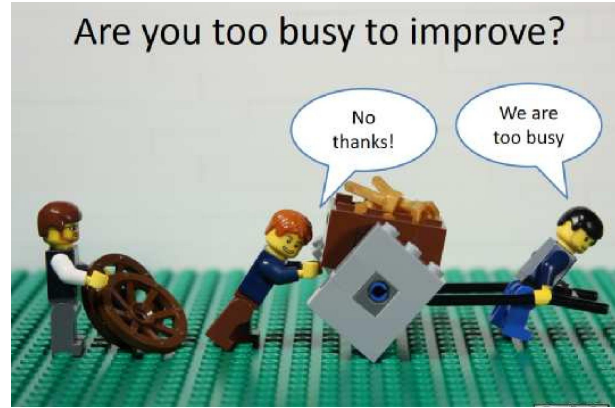
Desafíos (<10 años) en IA y Computación Científica

- Huella de Carbono. Algoritmos verdes. Sostenibilidad de los recursos, alargar su vida útil.
- Incorporar IA generativa y los Modelos de Lenguaje.
- Seguridad en la toma de decisión basada en IA robusta.
- Propagación de incertidumbre en Redes Neuronales.
- Redes Neuronales Informadas por la Física.
- Diseño de instrumentación científica guiado por IA.

- Impacto Social directo y a corto plazo.
- Formación en IA para otros profesionales: físicos de partículas, astrofísicos, ingenieros, oncólogos, personal de administración, etc.
- Atracción y retención de talento en IA.
- Explicabilidad es el punto de encuentro de dos disciplinas científicas.
- Estrategia Europea/Nacional de IA.

Resumen (muy personal)

- Los datos van a incrementar la velocidad de generación, complejidad y variedad.
- El valor y veracidad son más importantes que en el paso reciente.
- Las **redes neuronales** ofrecen capacidades únicas pero mal utilizadas si no van acompañadas de **explicabilidad** y **robustez** en las decisiones.
- La IA generativa supone un salto en los patrones de trabajo. **Mantener el control sobre los resultados.**
- La **huella de carbono** será un elemento esencial en el futuro.



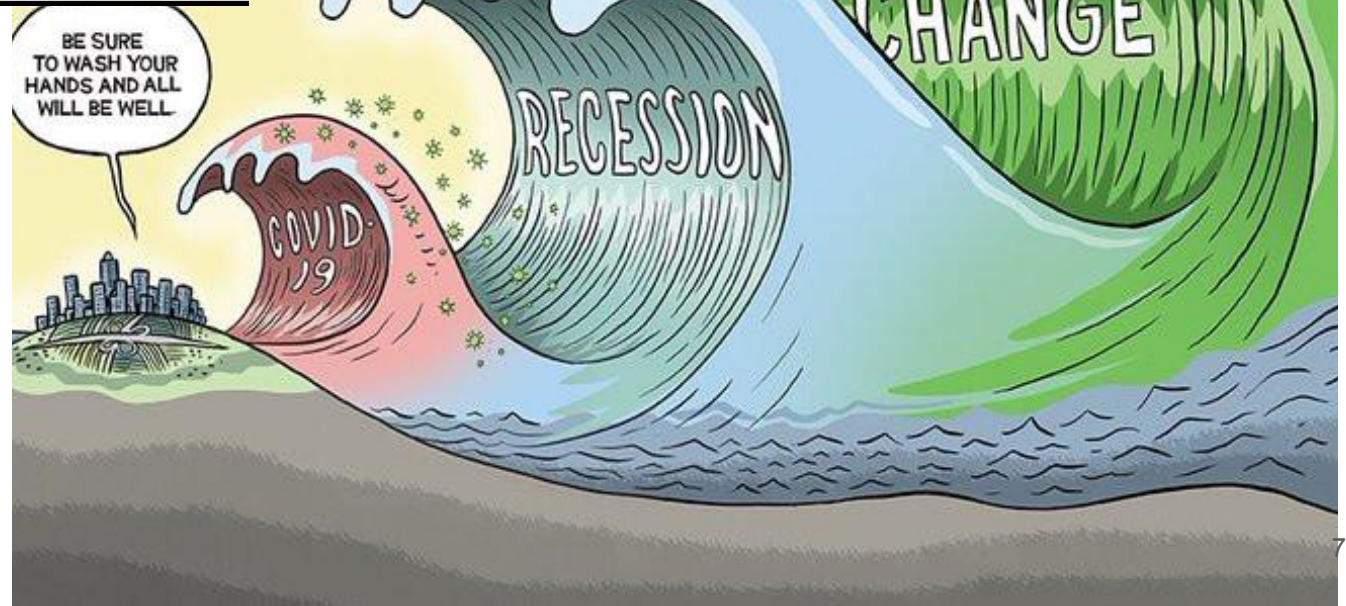
- + Computación
- + Matemática
- + Integración con el problema: física, etc.

Las divisiones las establecemos los humanos, no la naturaleza.



Mucha IA
para afrontar
los desafíos
futuros.

BE SURE
TO WASH YOUR
HANDS AND ALL
WILL BE WELL.



TFMs

<http://www.wae.ciemat.es/~cardenas/TFM.html>

- *Architectural Optimization of Dynamic Inception Modules in Convolutional Neural Networks using the Coral Reef Optimization Algorithm*, **David Pineda Peña**
- *Prediction Head Neck Cancer with Deep Active Learning*, **Enrique Arroyo Escribano**
- *Nature-Inspired Computation: two cases*, **Pedro García Victoria**
- *Segmentación automática de series temporales con algoritmos de aprendizaje no supervisado con aplicación a la calidad aire en Madrid*, **Alejandro Luque Cerpa**
- *Optimización Automática de Hiperparámetros en Modelos de Aprendizaje Automático mediante PBIL*, **Andrés Vasco Carofilis**
- *Técnicas de Deep Learning para la predicción de los niveles de contaminación*, **Juan Cañete Rodríguez**
- *Aplicaciones de aprendizaje: Modelado y Pronóstico de la Serie Temporal de ^{222}Rn en el Laboratorio Subterráneo de Canfranc*, **Iván Méndez Jiménez**