International Workshop on Machine Learning for Space Weather: Fundamentals, Tools and Future Prospects

7-11 November 2022
This is a hybrid meeting
Buenos Aires, Argentina

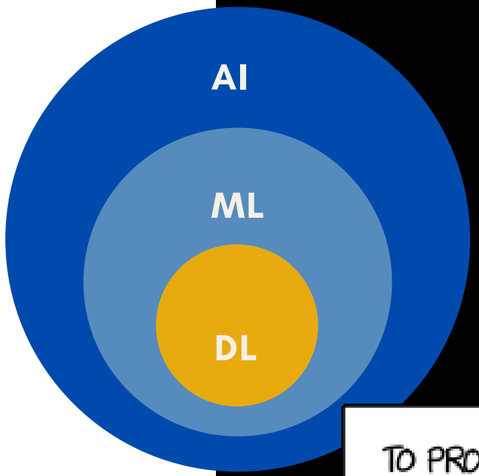
Further information:
https://indico.ictp.it/event/9840/
smr3750@ictp.it
+39-040-2240284
Elizabeth Brancaccio

Dra María Graciela Molina
FACET-UNT / CONICET
Tucumán Space Weather Center - TSWC

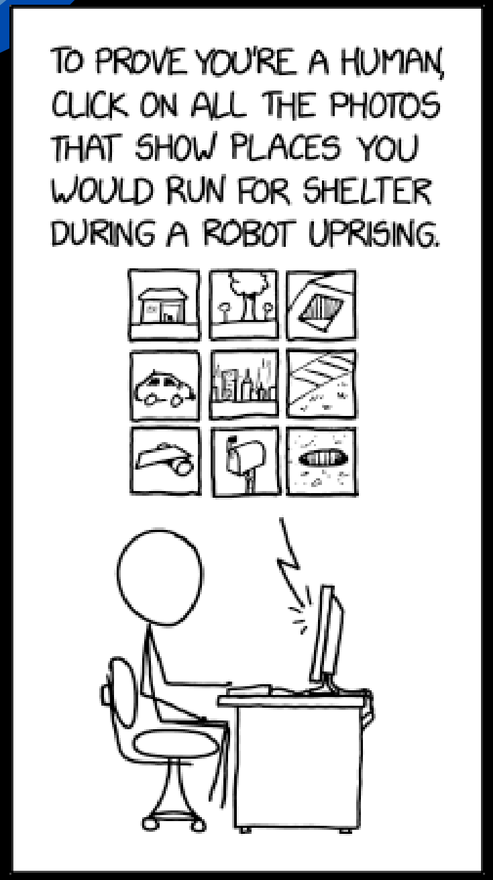
https://spaceweather.facet.unt.edu.ar/
IG -> @spaceweatherargentina

gmolina@herrera.unt.edu.ar

Deep Learning



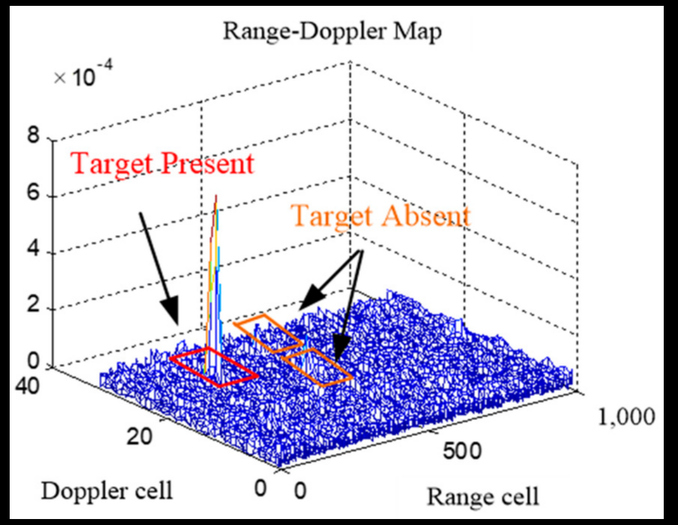
Extract patterns from data using neural networks

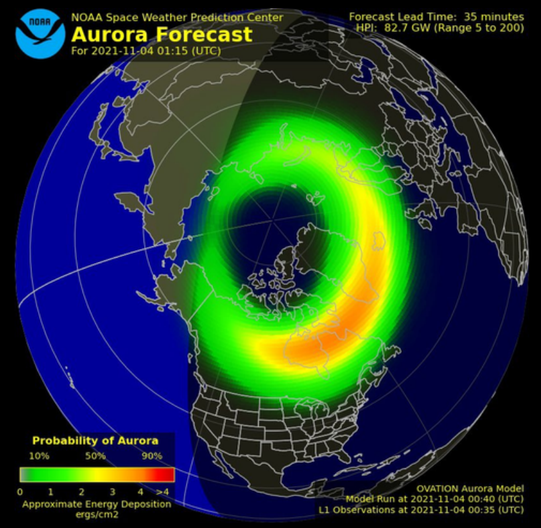


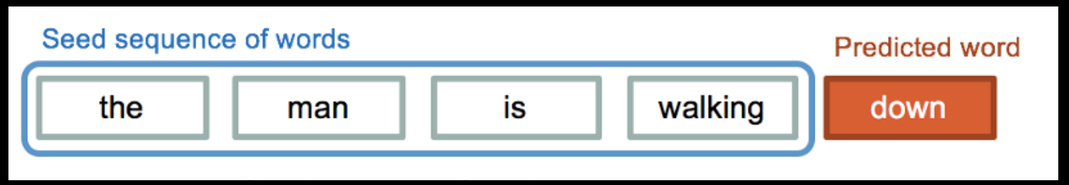
- https://this-person-does-not-exist.com/en

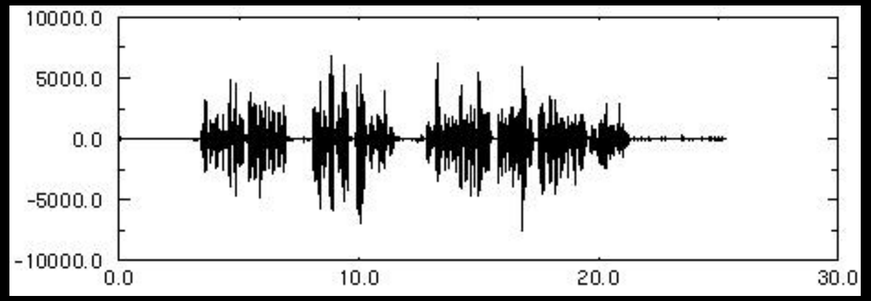
Recurrent Neural Networks

- Processing a sequence of data $x(t)= x(1), \ldots, x(\tau)$
- Recurrent -> perform the same task for every element of a sequence, with the output being depended on the previous computations.
- Have a “memory”









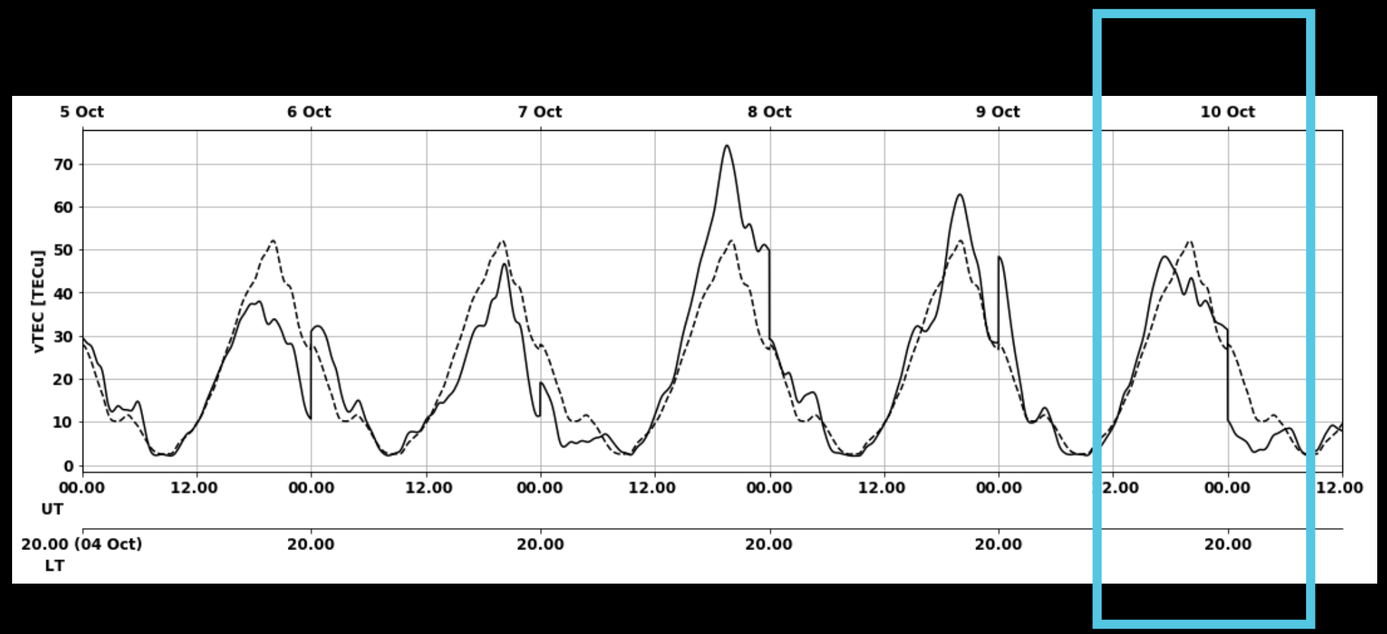
Recurrent Neural Networks

RNNs as an approach to sequence modeling problems

We want to forecast this

To model sequences, we need to:

- Handle **variable-lenght** sequences
- Track **long-term** dependences
- Mantain information about **order**
- **Share parameters** across the sequence



Recurrent Neural Networks

RNNs as an approach to sequence modeling problems

how many steps? (lenght)

To model sequences, we need to:

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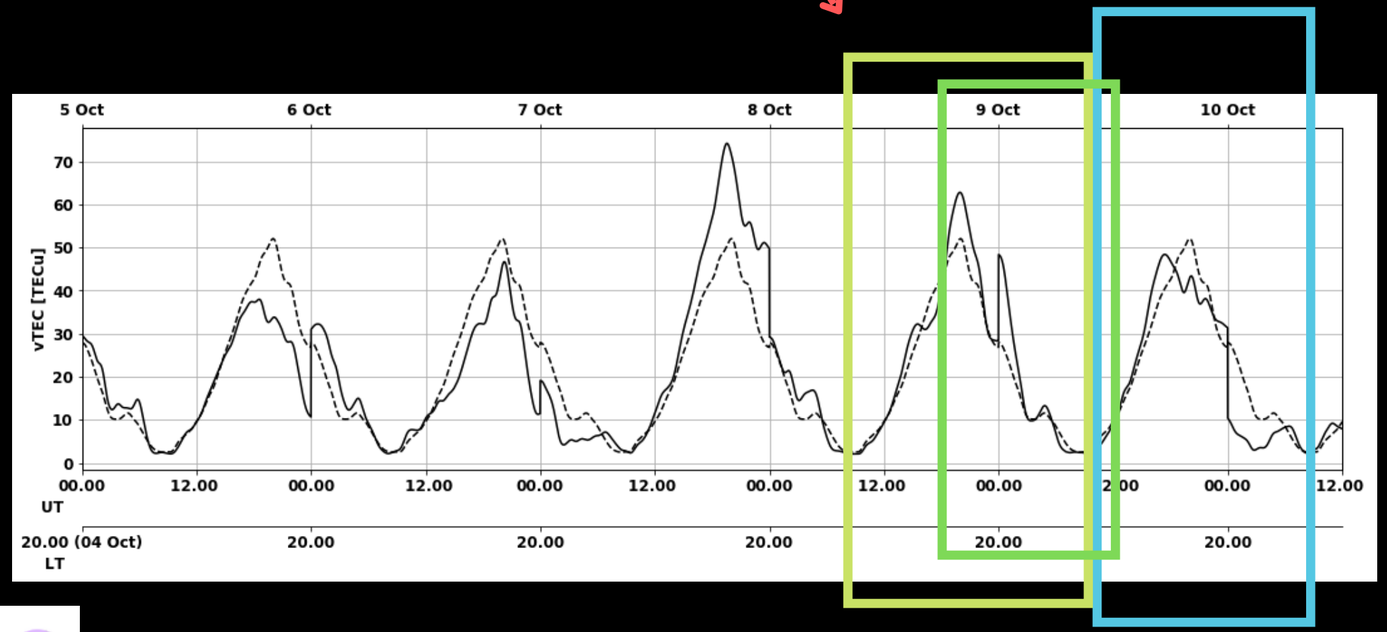

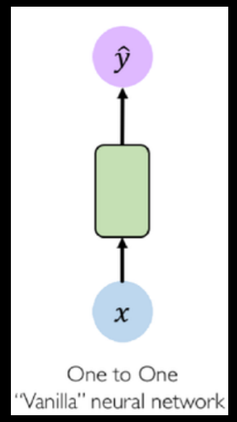

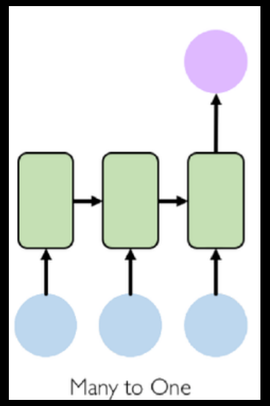

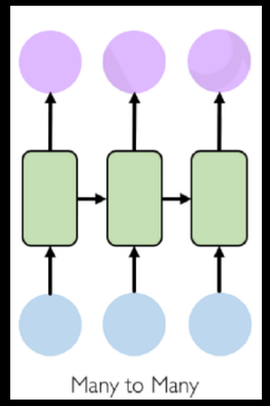

and more arquitecutes

Recurrent Neural Networks

RNNs as an approach to sequence modeling problems

how important is the information on the (far) past ?

To model sequences, we need to:

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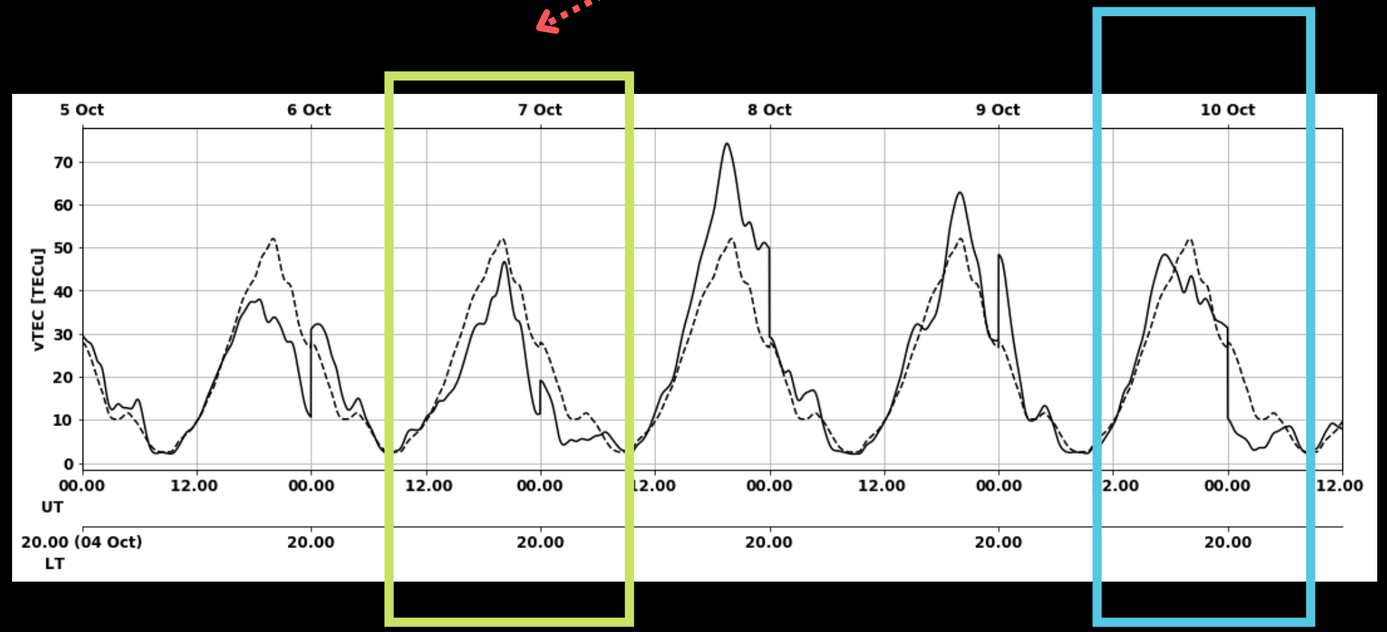

E.g. Ionosphere regular behaviour
(daily, seasonal, solar cycle, ...)

Recurrent Neural Networks

RNNs as an approach to sequence modeling problems

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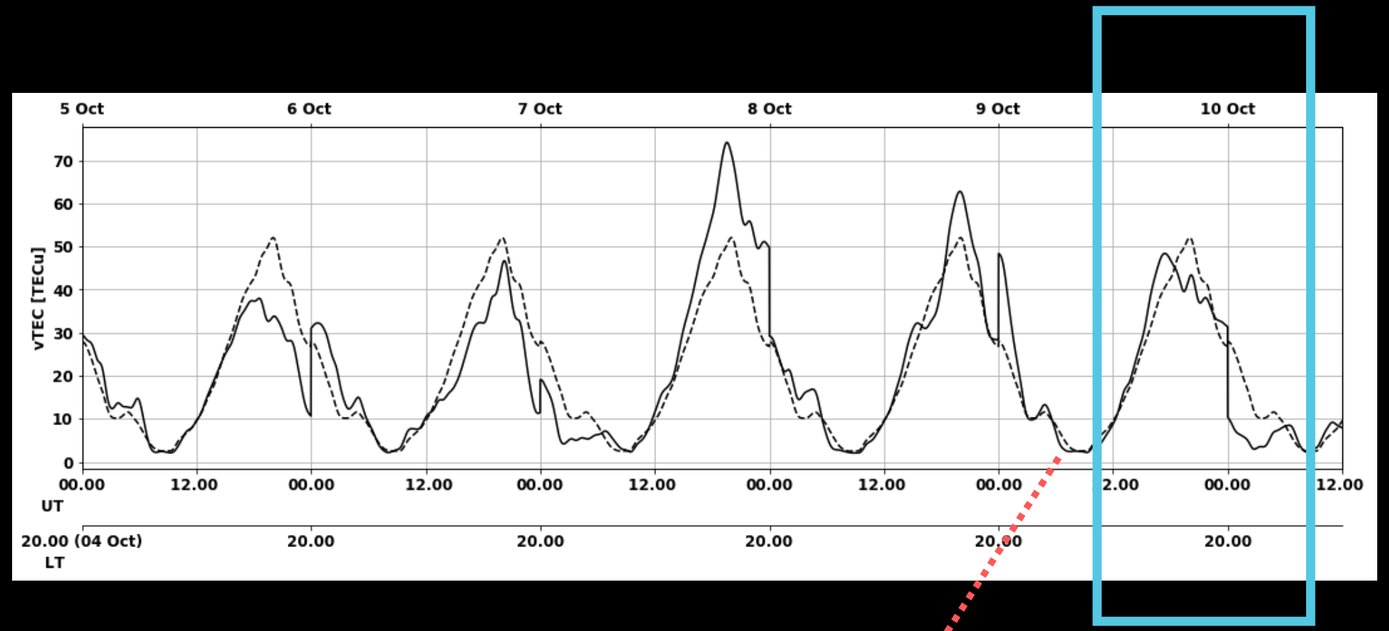

vTEC (t-2), vTEC (t-1), vTEC (t-0) <> vTEC (t-0), vTEC (t-2), vTEC (t-1)

Recurrent Neural Networks

RNNs as an approach to sequence modeling problems

To model sequences, we need to:

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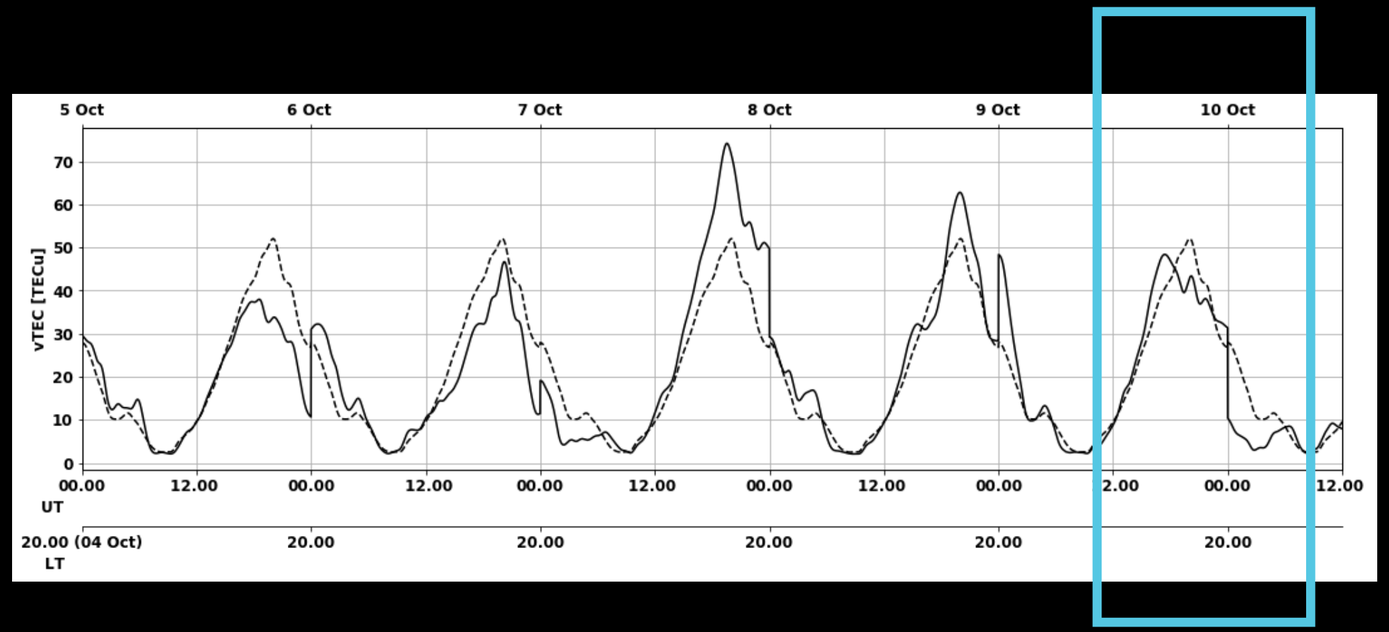
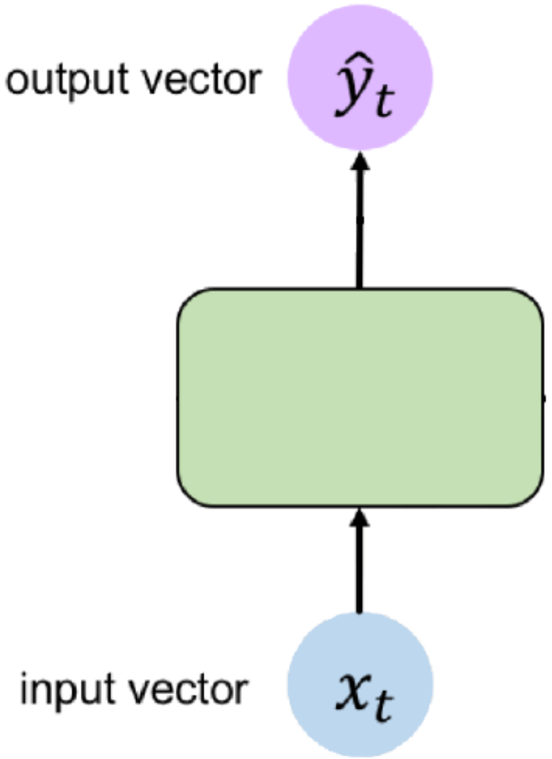
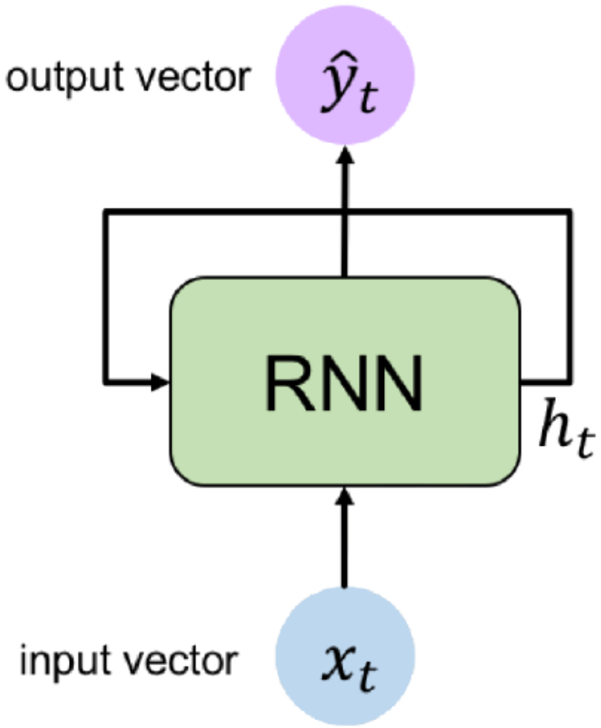
- Share parameters across the sequence



RNNs have a state (h_t), that is updated at each time as a sequence is processed using the same parameters each time step

Recurrent Neural Networks



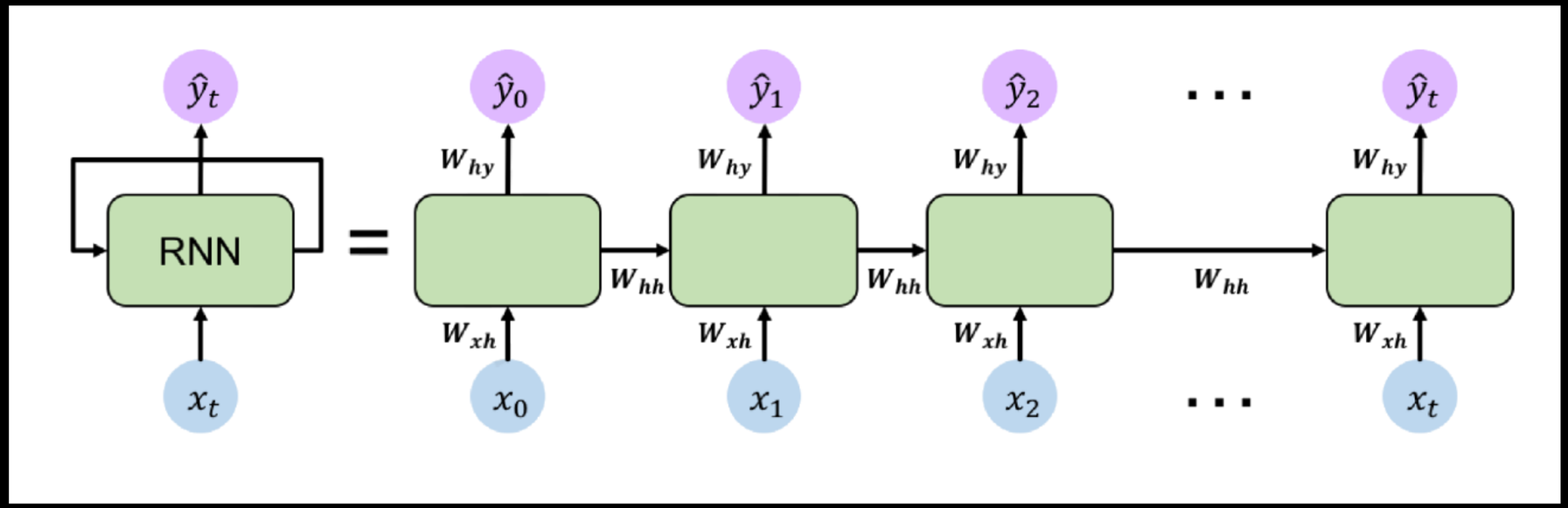


$$h_t = f_W(h_{t-1}, x_t)$$

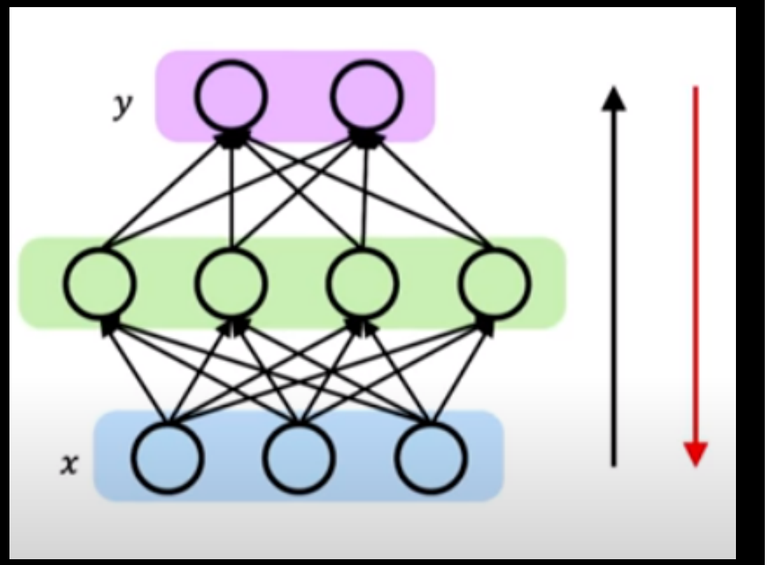
- h_t: cell state
- f_W: function parameterized by W
- h_{t-1}: old state
- x_t: input vector at time step t

Apply a recurrent relation at every time step to process a sequence

Recurrent Neural Networks



Backpropagation through time: long time dependences



$$W^* = \underset{W}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}\left(f\left(x^{(i)}; W\right), y^{(i)}\right)$$

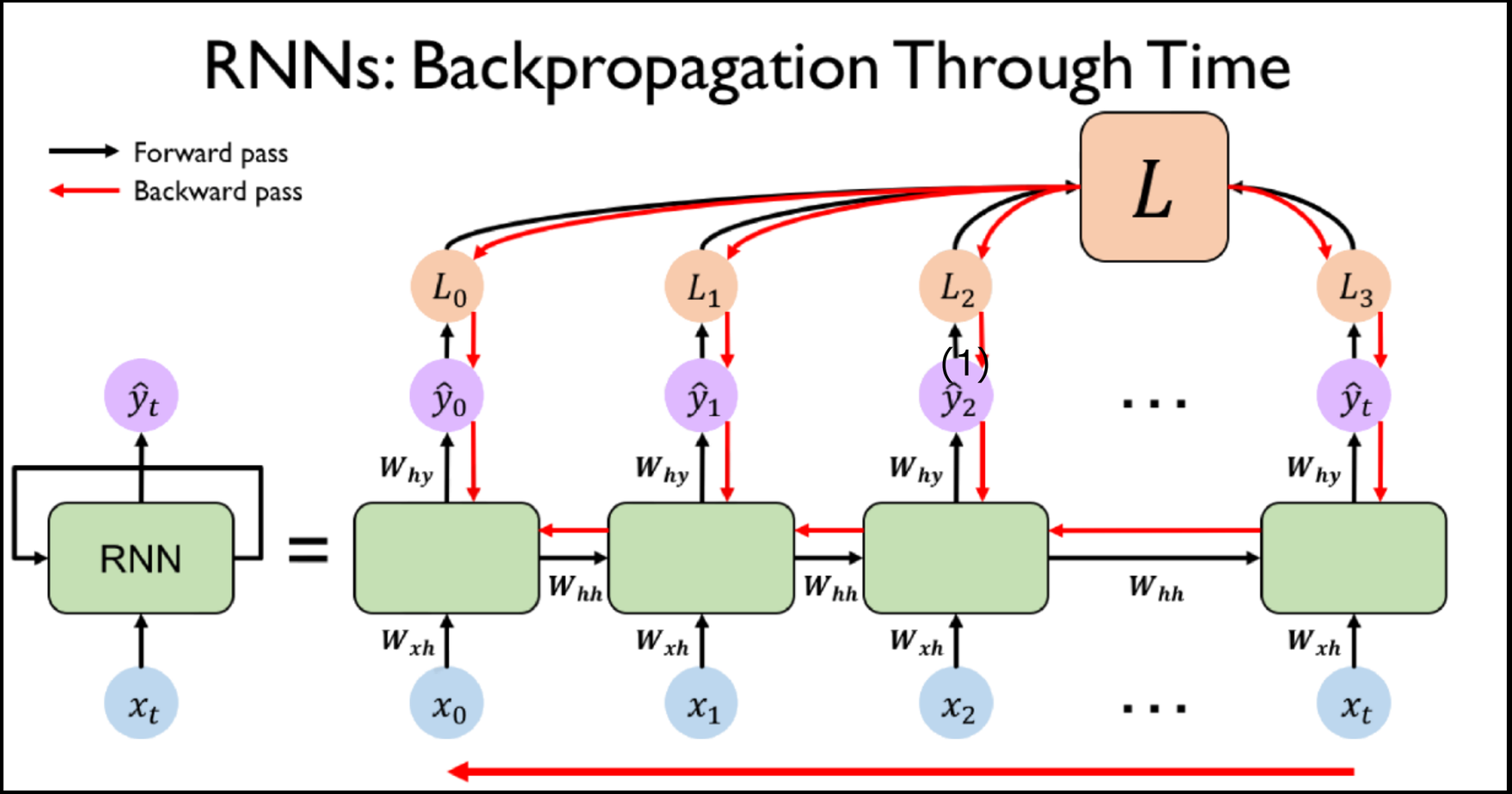
$$W^* = \underset{W}{\operatorname{argmin}} J(W)$$

Algorithm

1. Initialize weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Compute gradient, $\frac{\partial J(W)}{\partial W}$
4. Update weights, $W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$
5. Return weights

- take the gradient of loss with respect to each parameter
- shift parameters in order to minimize loss

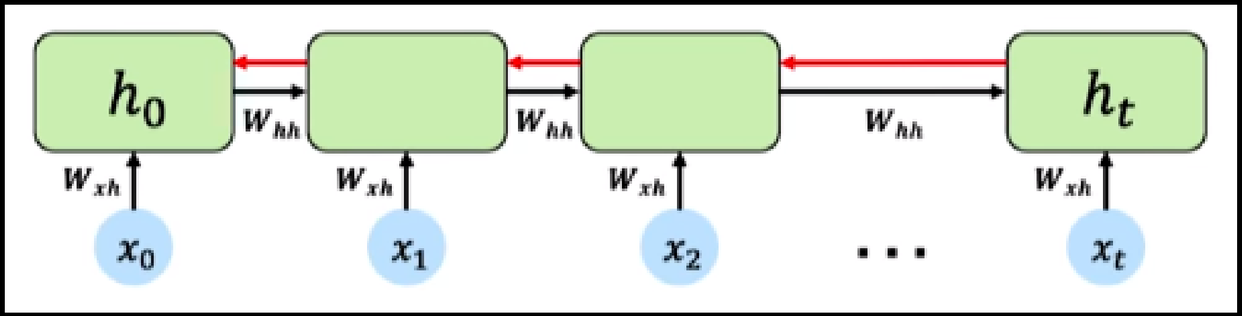
Backpropagation through time: long time dependences



- Compute individual l_i for individual time steps and sum them
- Backpropagate errors individually for each time step and then to all the time steps to the beginning of the sequence.

https : //kharshit.github.io/blog /2019/02/22/backpropagation – through – time

Backpropagation through time: long time dependences



- high computation time!

- Many values >>1 -> exploding gradient (*)
- Many values <<1 -> vanishing gradient

(*) Gradient clipping is a simple technique: If the gradient gets too large, we rescale it to keep it small.

Vanishing gradient problem

Multiply many small numbers together

Errors due to further back time steps have smaller and smaller gradientes

Bias parameters to capture short -term dependencies

How to tackle the problem:

- Activation function
- Weight initialization
- Network architecture

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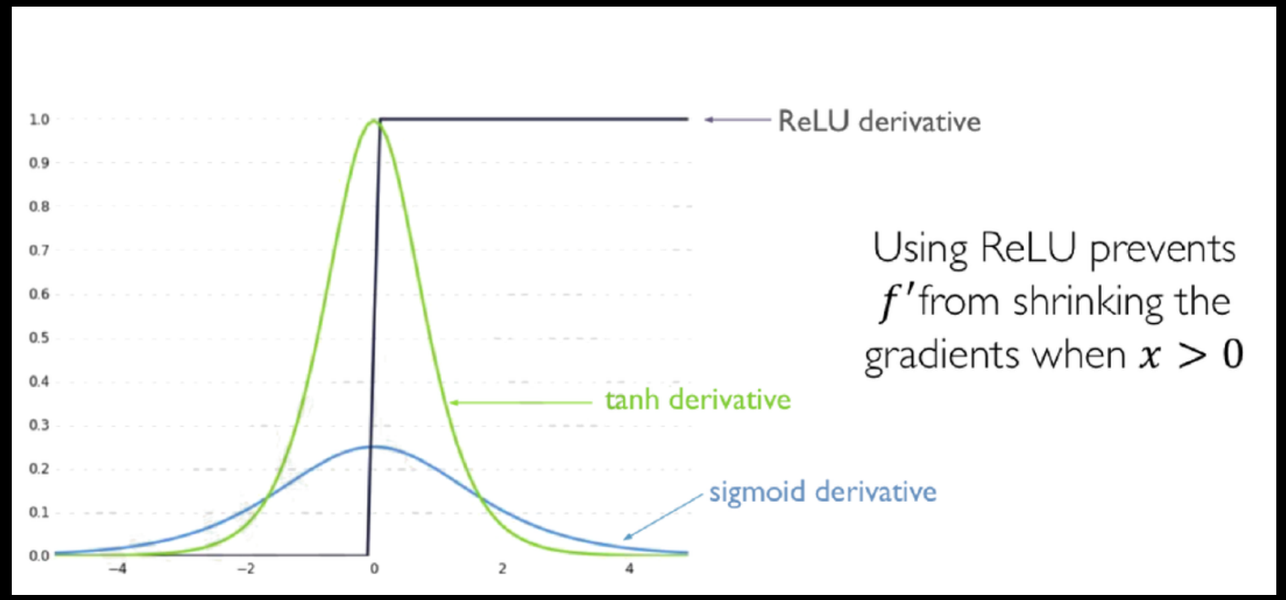

Vanishing gradient problem

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Errors due to further back time steps have smaller and smaller gradientes

Bias parameters to capture short -term dependencies (we "loose" long-term dependencies)

How to tackle the problem:

- Activation function
- Weight initialization
- Network architecture

$$I_n = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}$$

Initialize weigths to identity matriz
Initialize biases to zero

prevent the weights to shrinking to zero

Vanishing gradient problem

Multiply many small numbers together

Errors due to further back time steps have smaller and smaller gradientes

Bias parameters to capture short -term dependencies (we "loose" long-term dependencies)

How to tackle the problem:

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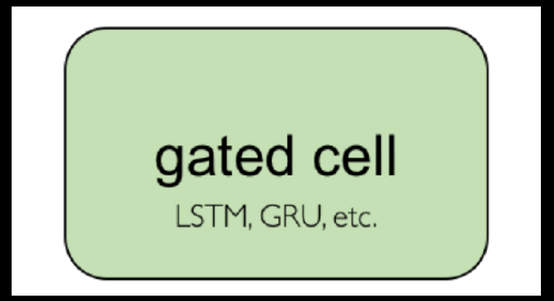
- Weight initialization
- Network architecture

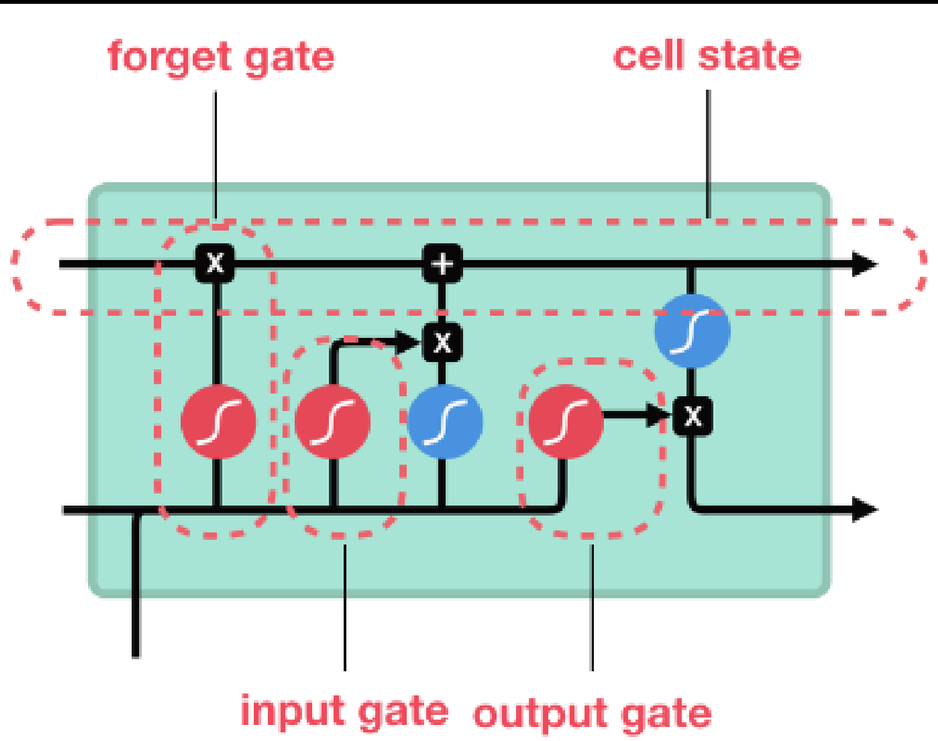
more rubust solution



- Use a more complex recurrent unit with gates to control what information is passed through.
- gates selectively add or remove information within each recurrent uniit

Long short term memory (LSTM)

Gates: 1) Forget 2) Input (store) 3)Update 4) Output



How it works:

1)Maintain a cell state
2)Use gates to control the flow of information

- Forget gate gets rid of irrelevant information
- Store relevant information from the current input
- Selectively update cell state

Output gate returns a filtered version of the cell state
3) Backpropagation TT with partially uninterrupted gradient flow

Long short term memory (LSTM)

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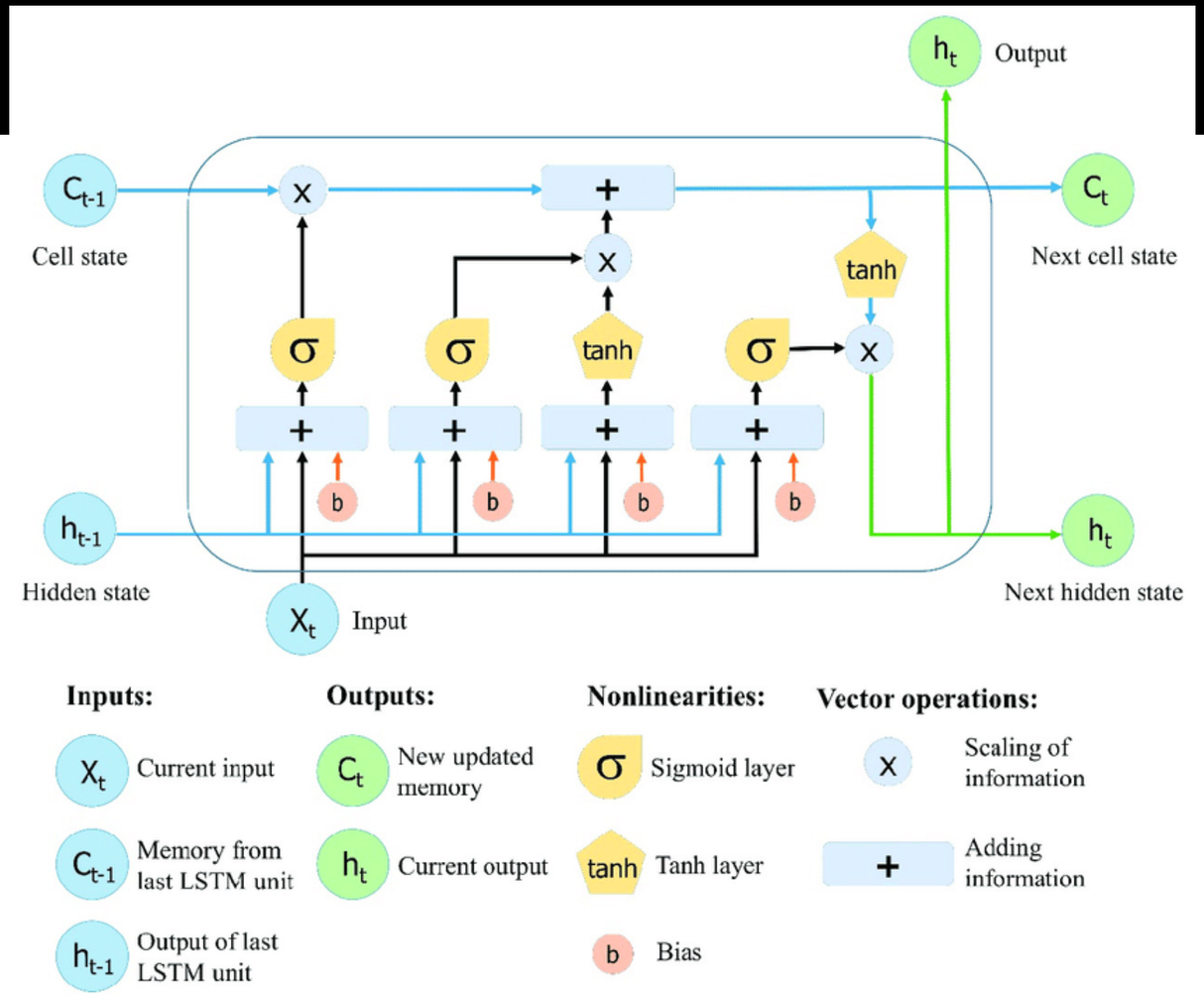

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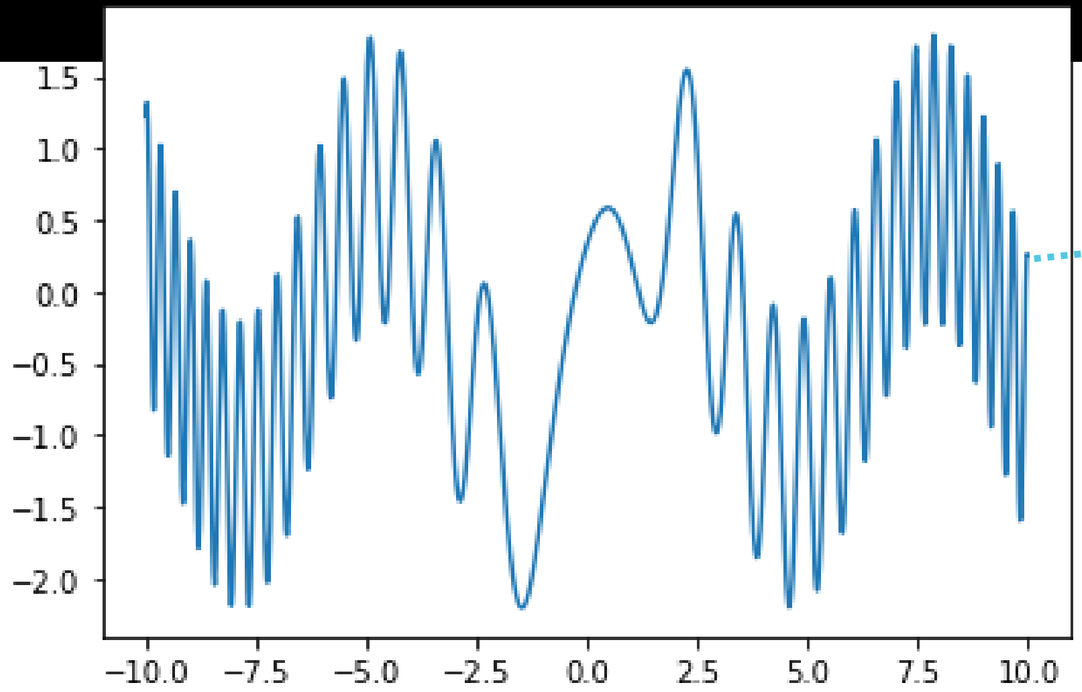
LSTM "not all that glitters is gold"

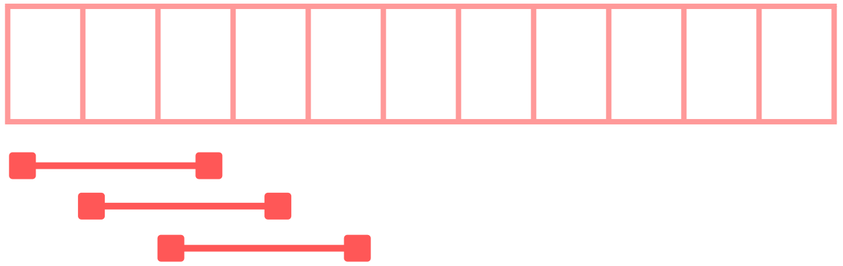
- << vanishing gradient problem .... but it doesn't completely remove it.
- >> computational resources
- affected by different random weight initialization
- Drop-out difficult to implement
- Prone to overfitting
- << performance for very long time problems

LSTM example

vanilla LSTM



training set t in [-10, 10)
test set t=10



the training set is an array of sequences (len = 3)

Convolutional Neural Networks

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Automated Individual Pig Localisation, Tracking and Behaviour Metric Extraction Using Deep Learning

JAKE COWTON[1,2], ILIAS KYRIAZAKIS[2], AND JAUME BACARDIT[1]
[1]School of Computing, Newcastle University, Newcastle upon Tyne NE1 7RU, U.K.
[2]School of Natural and Environmental Sciences, Agriculture, Newcastle University, Newcastle upon Tyne NE1 7RU, U.K.
Corresponding author: Jake Cowton (j.cowton2@newcastle.ac.uk)

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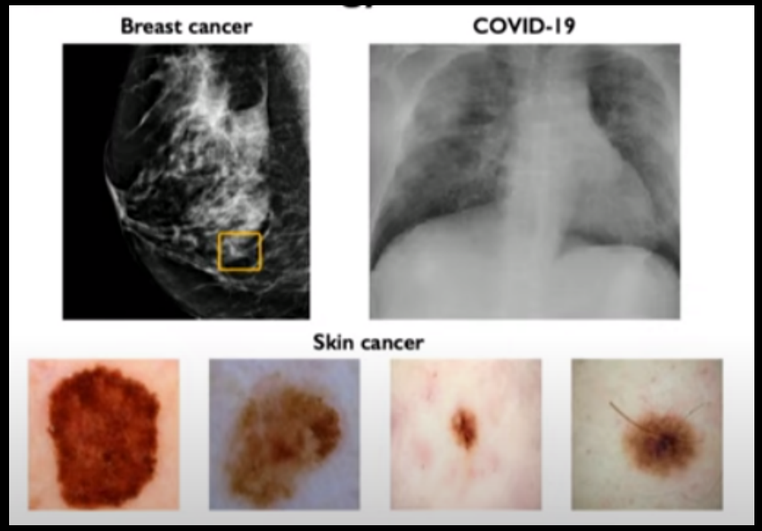
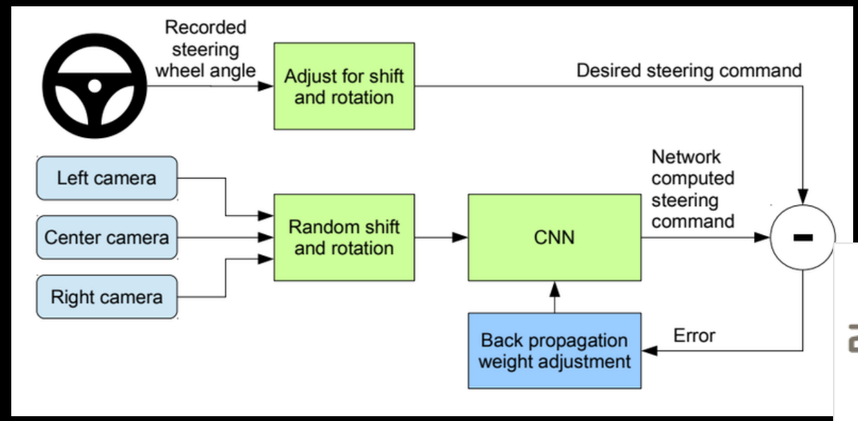
FIGURE 8. Four sample images from our pig detection test set processed by the Faster R-CNN with the feature extraction layers pre-trained on ImageNet, the rest pre-trained on Pascal Visual Object Classes Challenge 2007 and an additional fully-connected layer for the pig dataset. Detections to the left of the red wall are ignored. The top left image is from the low-light test segment. The top right image is from the densely packed test-segment. The bottom left image is from the overexposed test segment. The bottom right image is from the many pigs test segment.





Computer Vision. Some applications:

- Facial detection and recognition
- Healthcare, medicine and biology
- Self-driving vehicles

End to End Learning for Self-Driving Cars

We trained a convolutional neural network (CNN) to map raw pixels from a single front-facing camera directly to...

arXiv.org

Convolutional Neural Networks

Computer Vision. Some applications:

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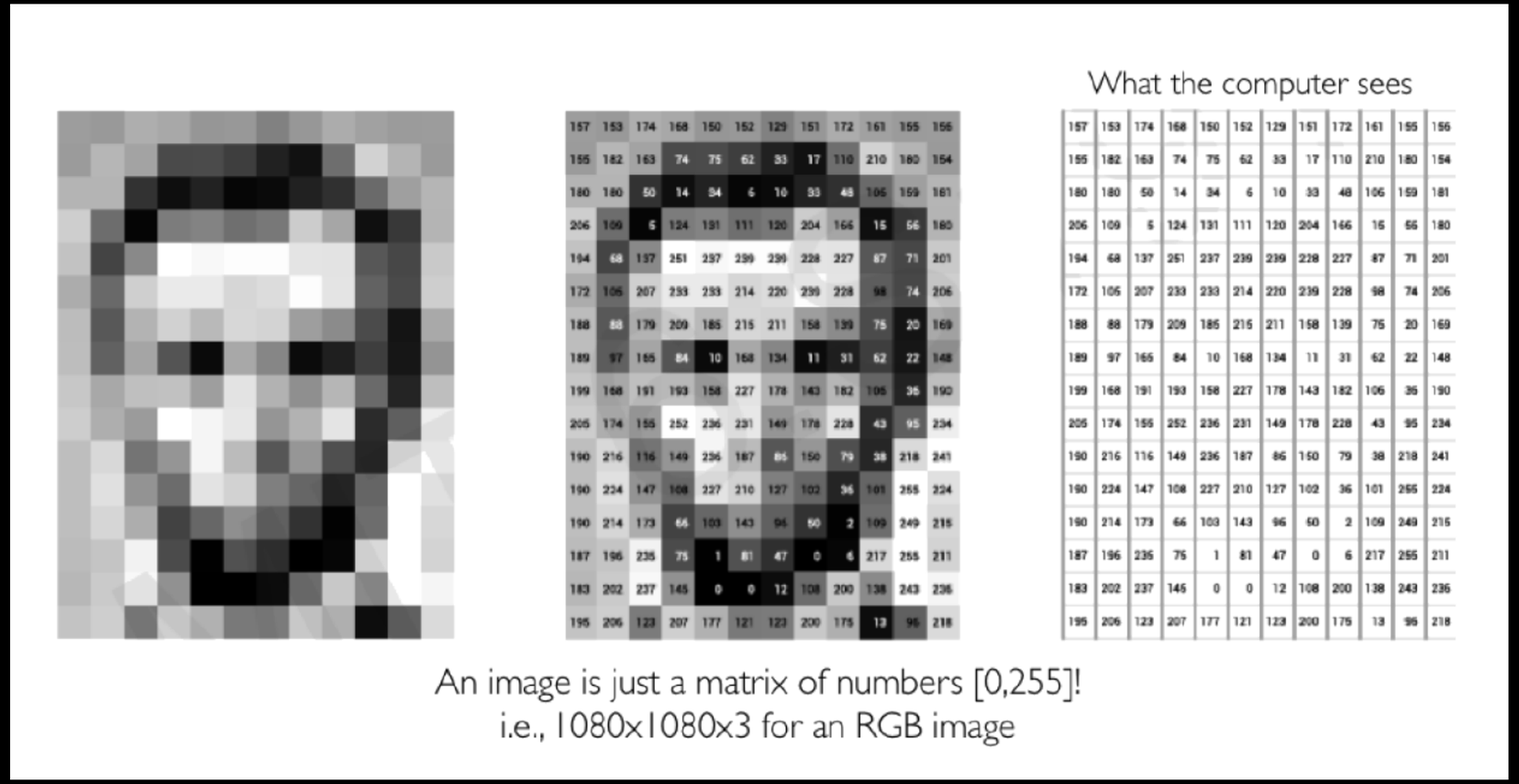
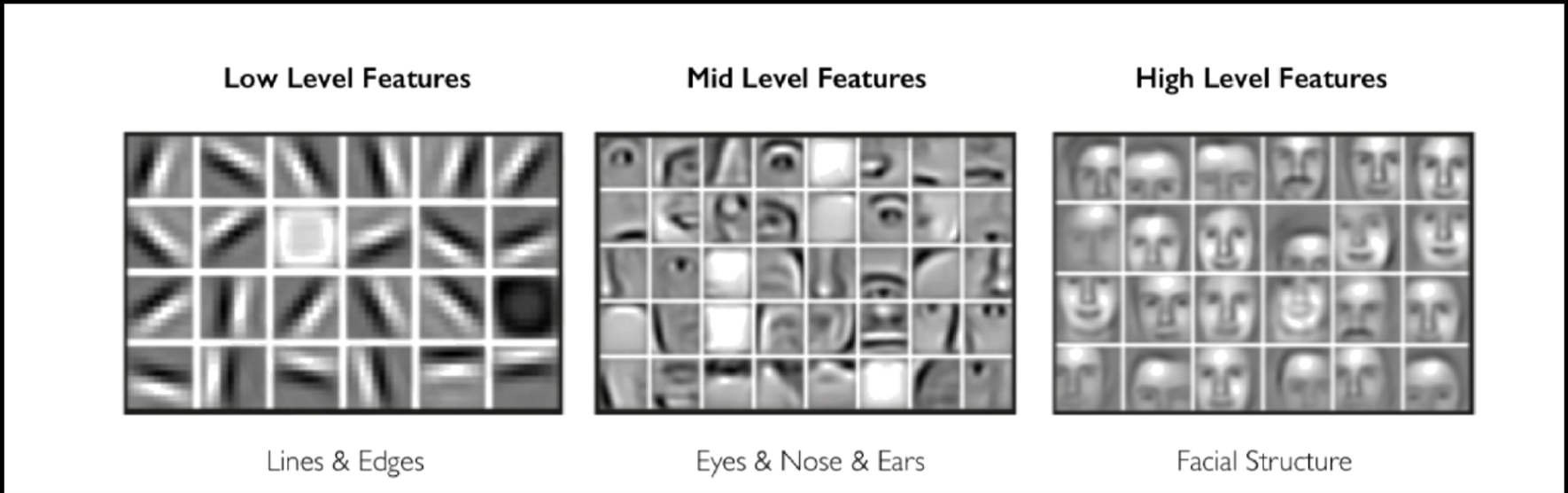


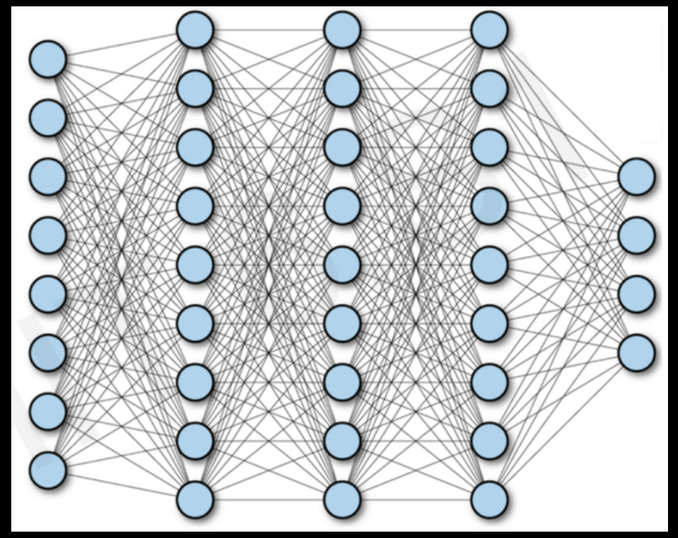
Features

(As in other NN problems)
- Regression
- Classification
- High level feature detection



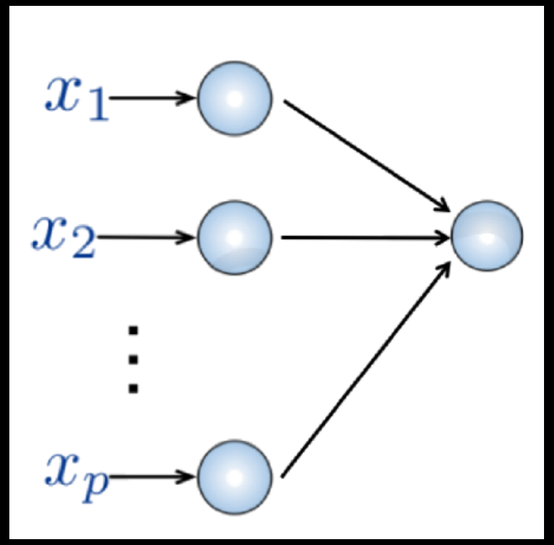
feature extraction from the data!
Learn hierarchy of features!

Fully connceted NN



Input:
- 2D image
- vector of pixel values

(flatten the image)



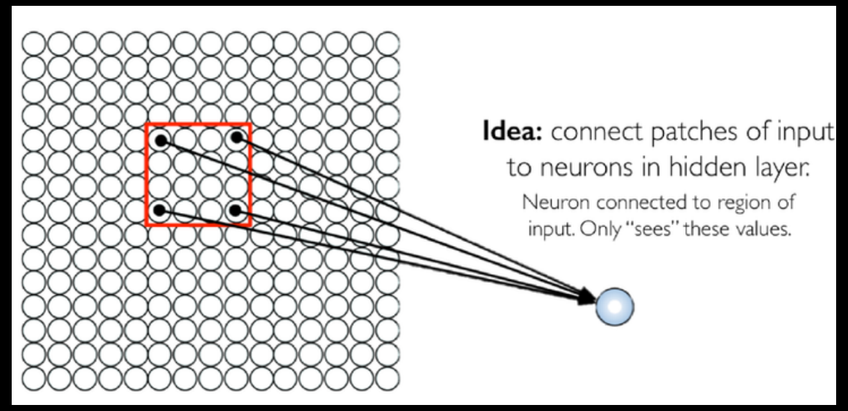
Fully connected:
- Connect neuron in hidden layer to all neurons in the input layer
- No spatial information!
- Lot of parameters

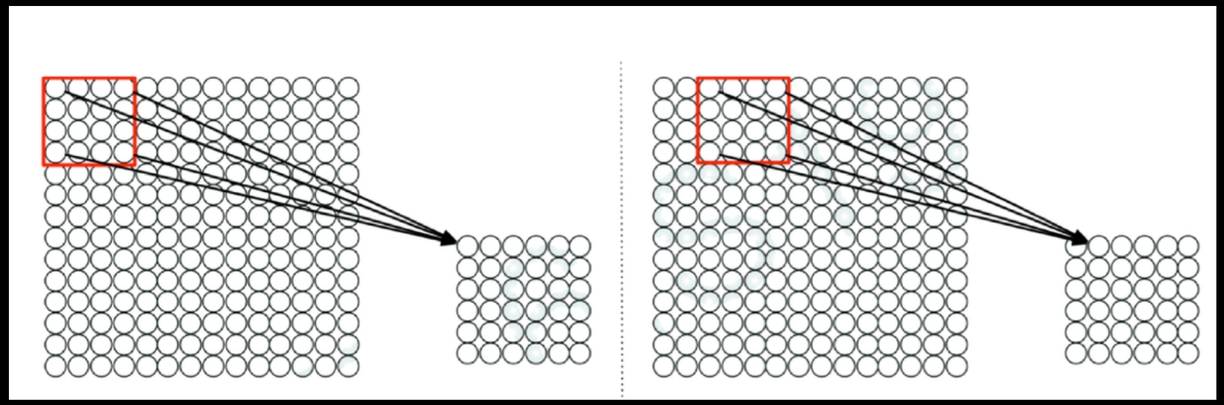
How to add spatial structure in the input?

Using spatial structure

Input:

- 2D image
- Array of pixel values

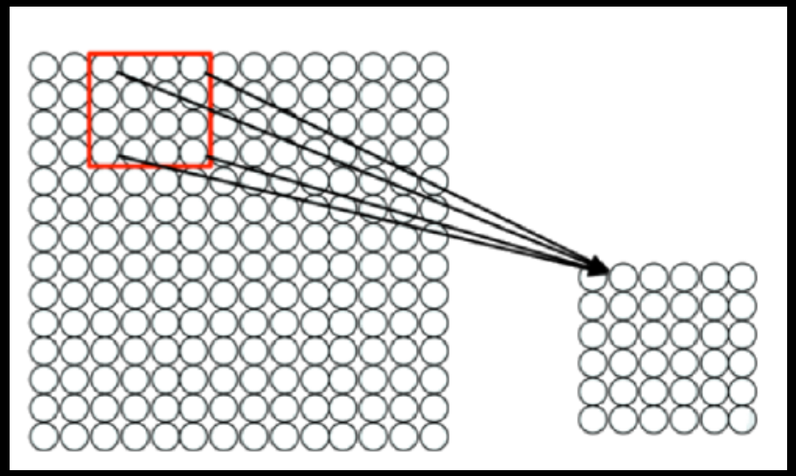




Sliding window to define conections,(connect patch in input layer to a single neuron)

The key: how can we weight the patch to detect particular features?

Using spatial structure

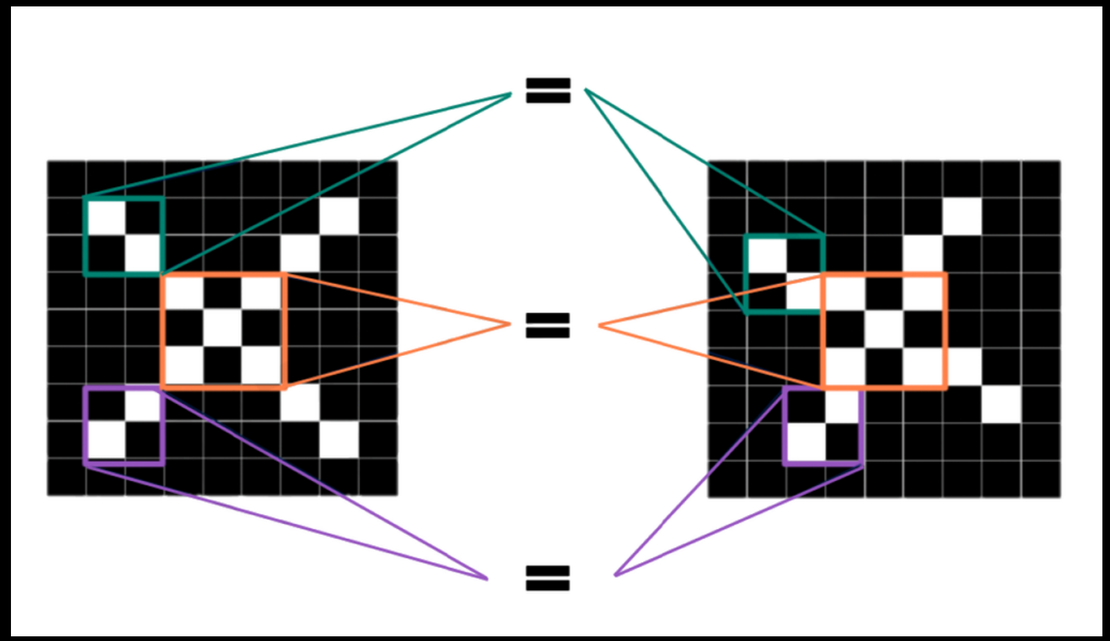


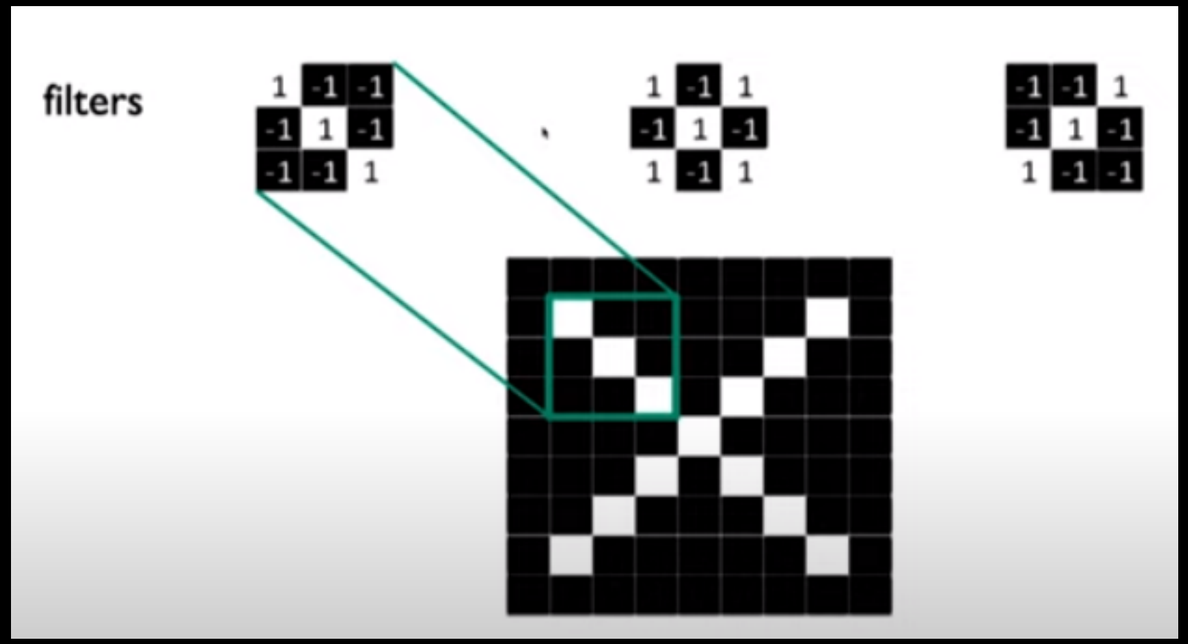
- Filter of size 4x4: 16 different weights
- Apply this same filter to a 4x4 patches in input
- Shift by 2 pixels for next patch

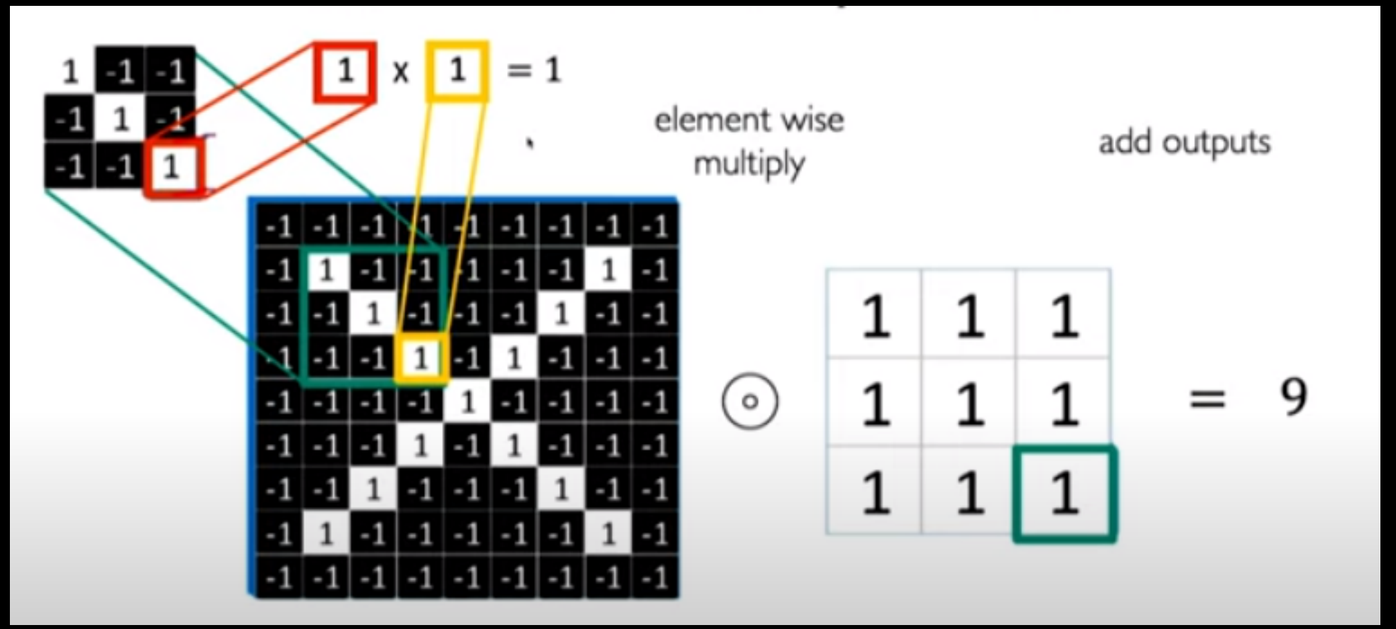
This "patchy" operation is convolution

- Apply a set of weights (a filter) to extract local features
- Use multiple filters to extract different features
- Spatially share parameters of each filter

Convolutional operation

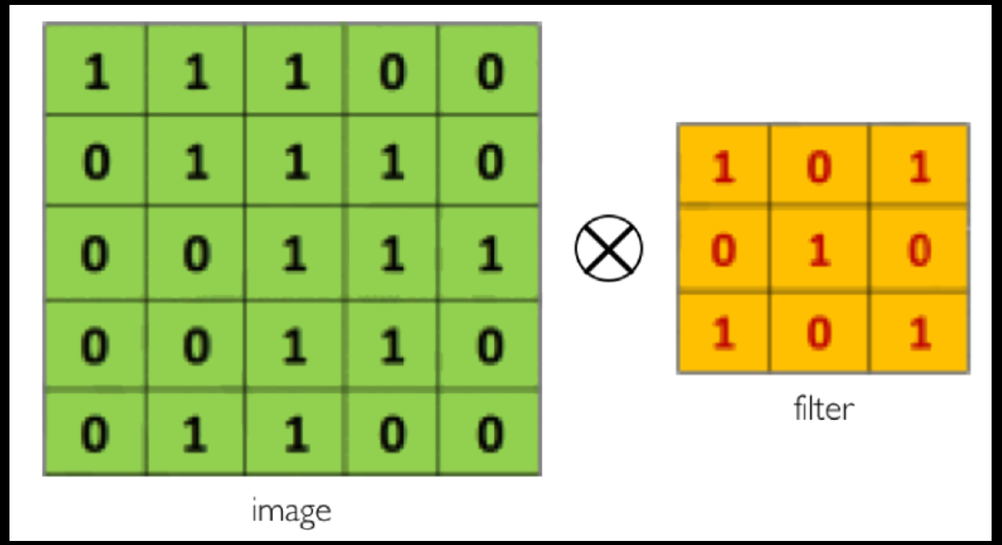


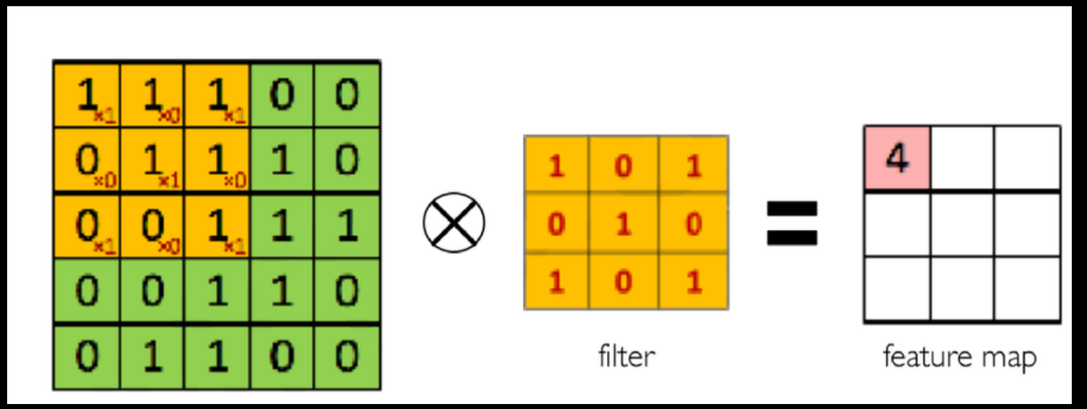


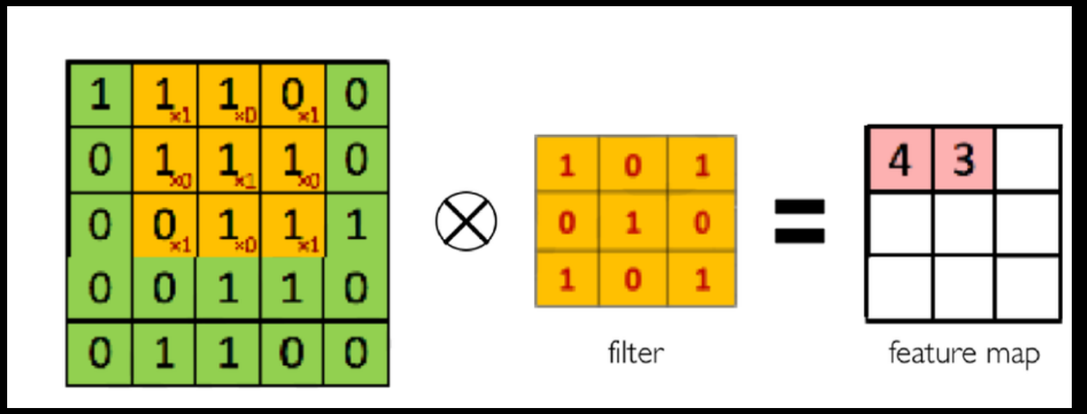


TSWC, 2022

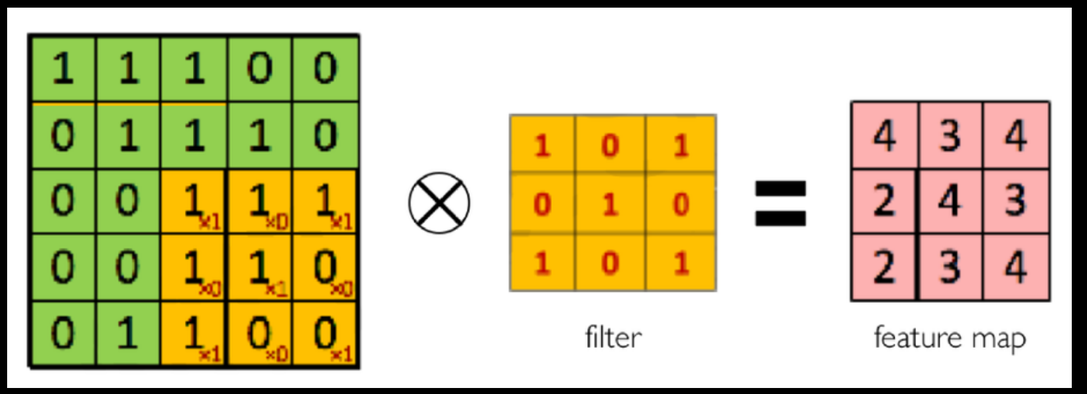
Convolutional operation





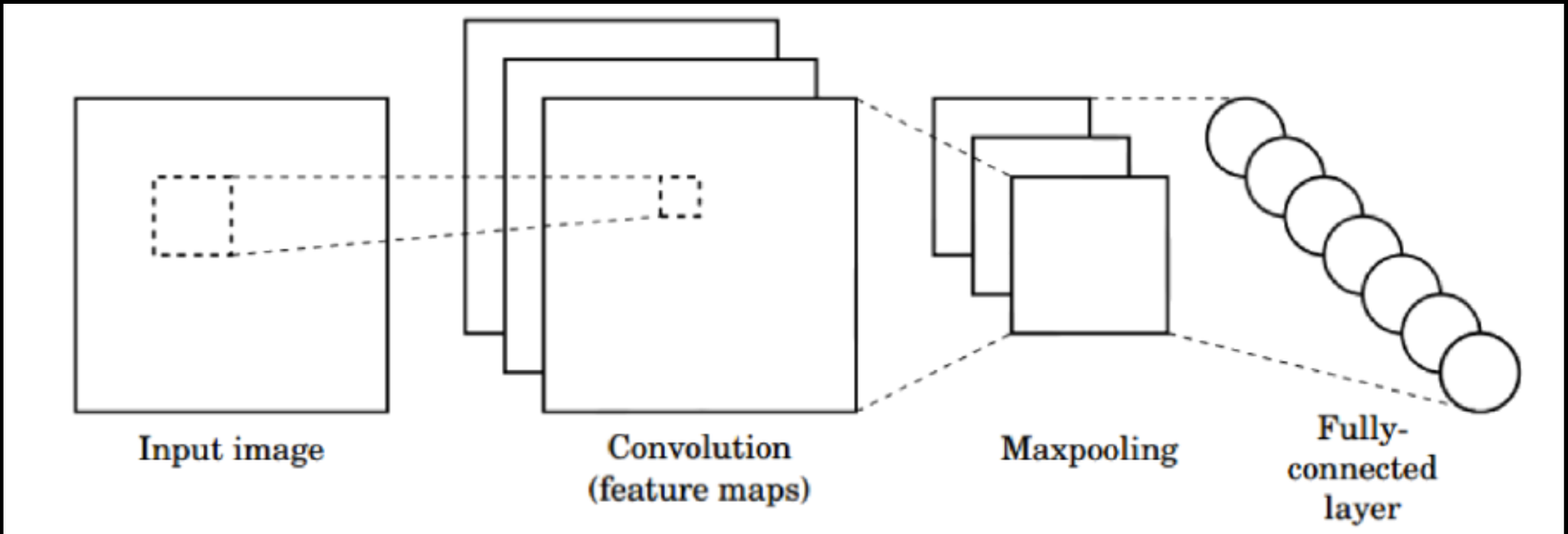


...



Convolutional neural networks (CNN)

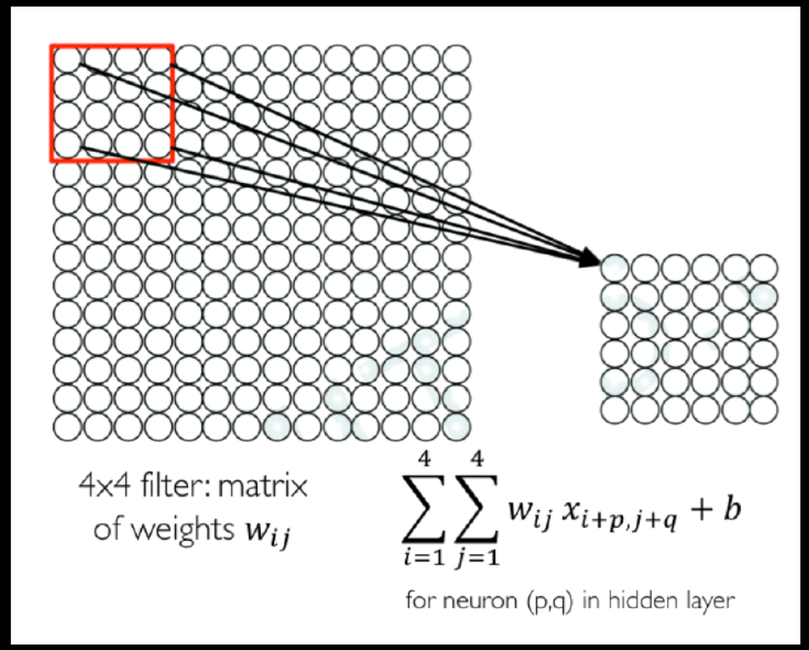
- for classification



- Convolution: apply filters to generate feature maps
- Non-linearity: often ReLU
- Pooling: Downsampling operation on each feature map

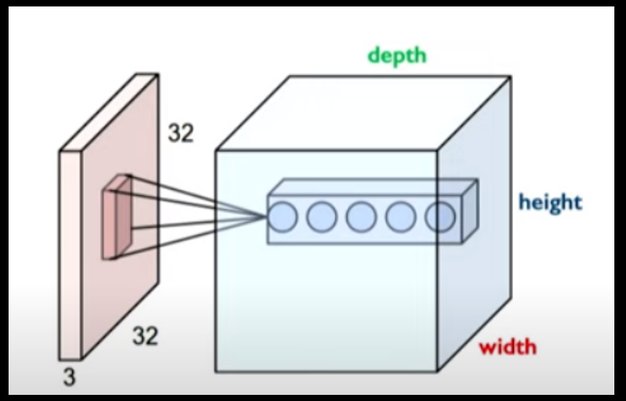
Train model with image data.
Learn weights of filters in convolutional layers.

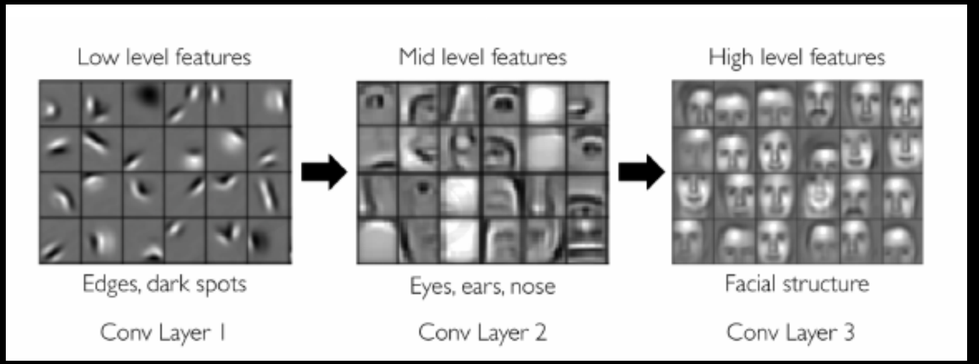
Convolutional layer



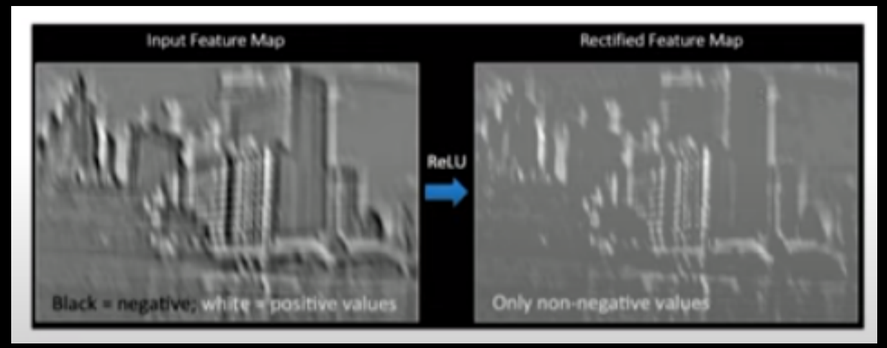
1. applying a window of weights
2. computng linear combinations

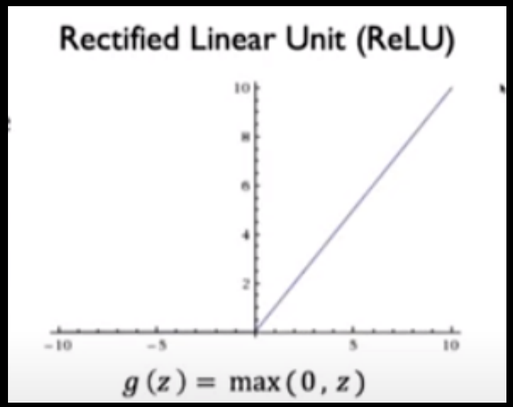
For a neuron in hidden layer
- Take inputs from patch
- Compute weighted sum
- apply bias



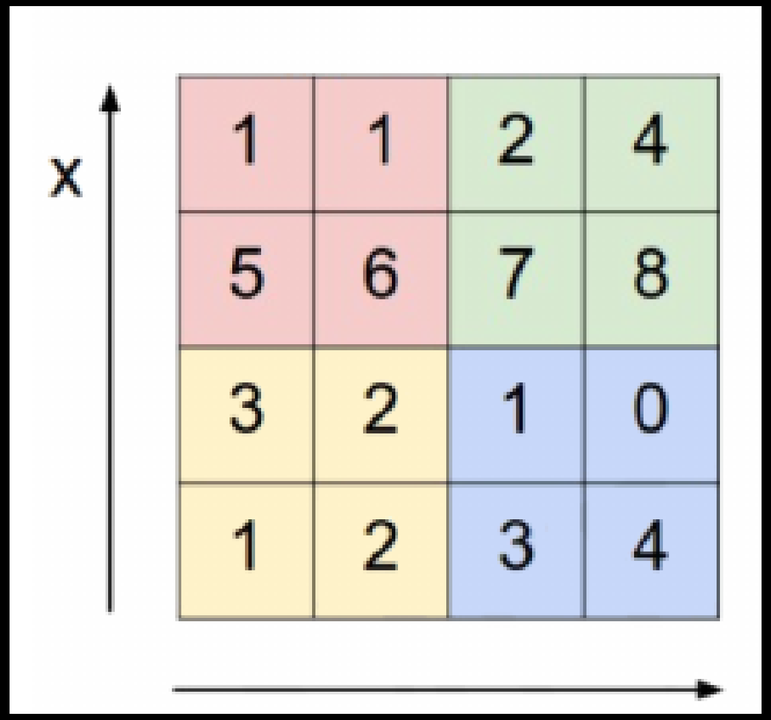


3. activating with non-linear function





Pooling

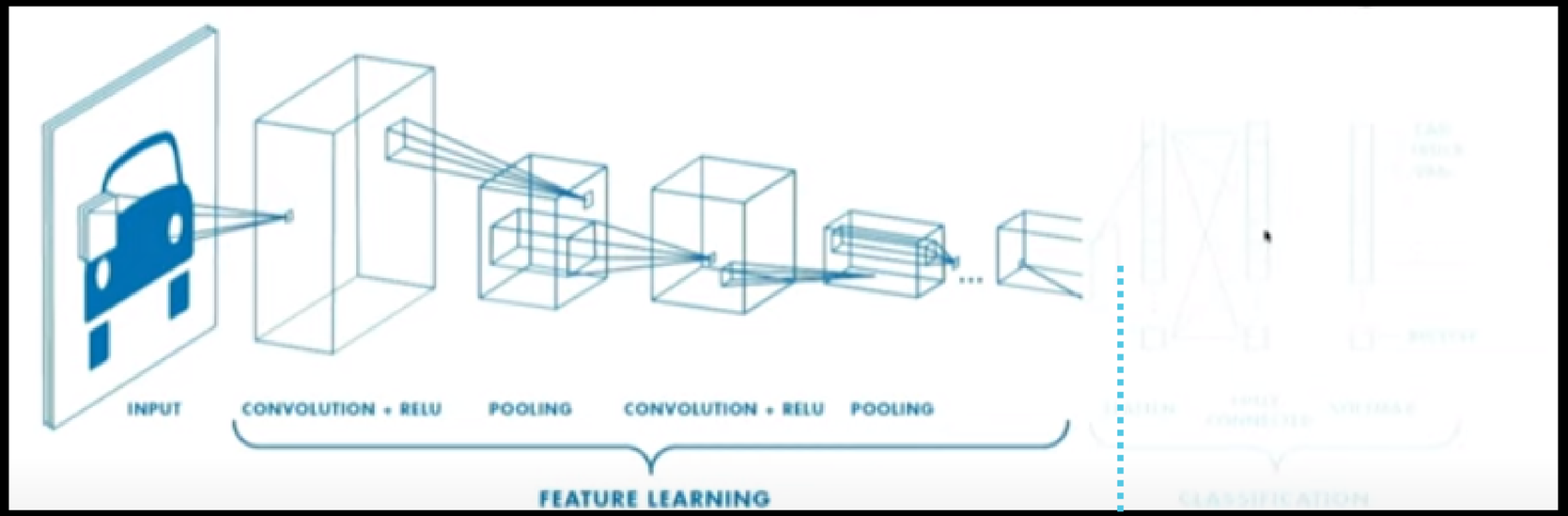


max pool with 2x2 filters
and stride 2

6	8
3	4

- Reduce dimensionality
- Spatial invariance

CNN: classification example

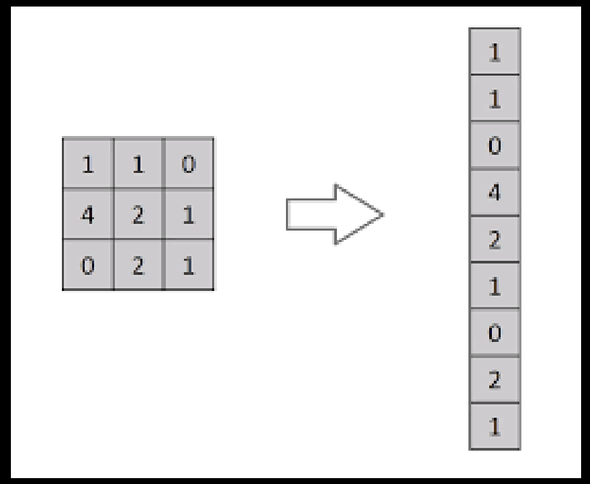


- Learns features in input image throught convolution
- Introduce non-linearity (activation func)
- Reduce dimensionality and preserve spacial invariance (pooling)

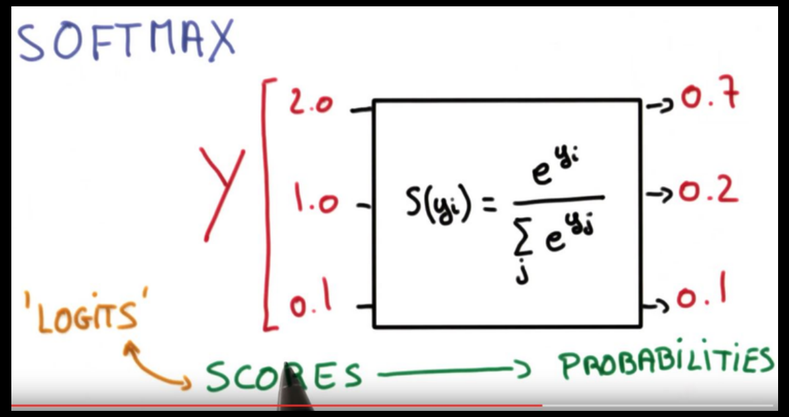
- at this point the last outpus is the i-th feature map

CNN: classification example

- CONV and POOL layers putput high-level features input
- Fully connected layer uses these features to classifying input image
- Express output as probability (image to certain class)



$$\text{softmax}(y_i) = \frac{e^{y_i}}{\sum_j e^{y_j}}$$



logits = unnormalised (or not-yet normalised) predictions (or outputs) of a model

HANDS-ON LAB

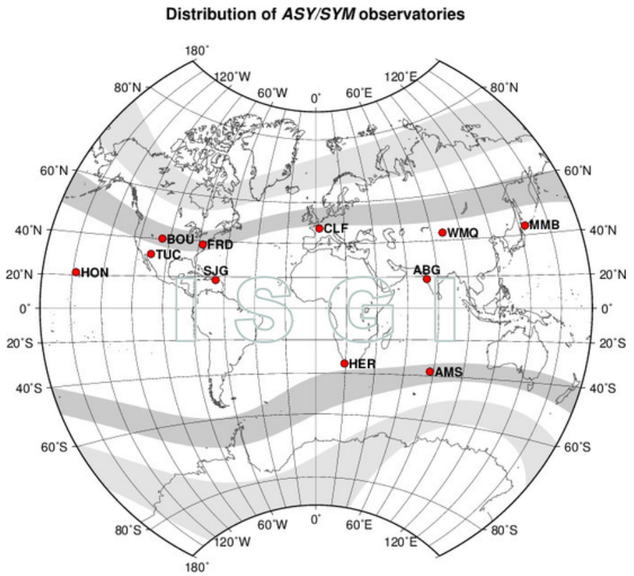
TP - 3

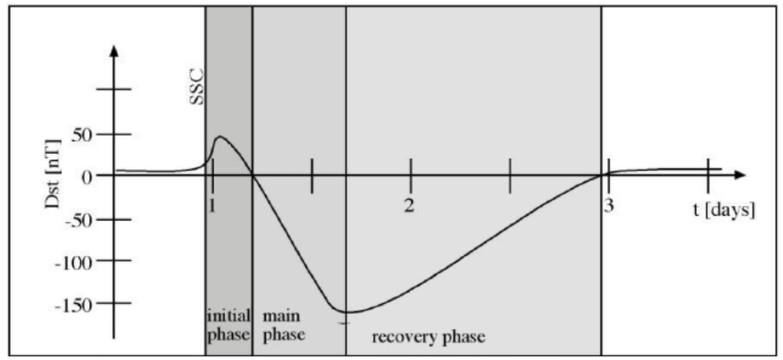
Sym-H forecasting

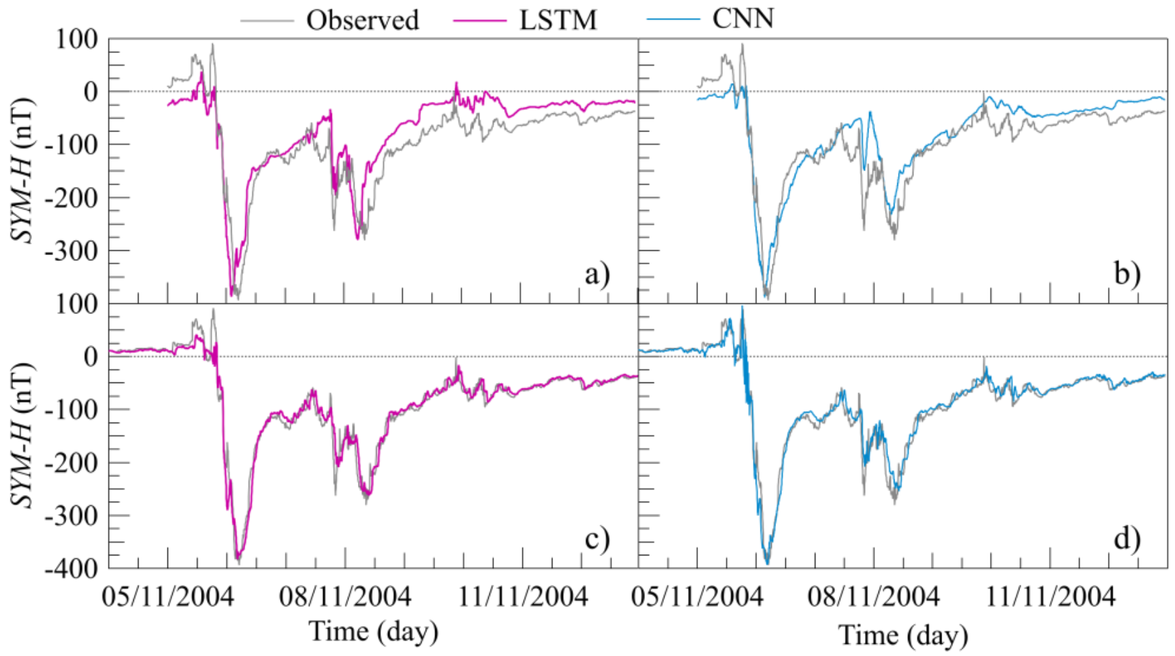
TSWC, 2022

From science to data science

http://isgi.unistra.fr/indices_asy.php





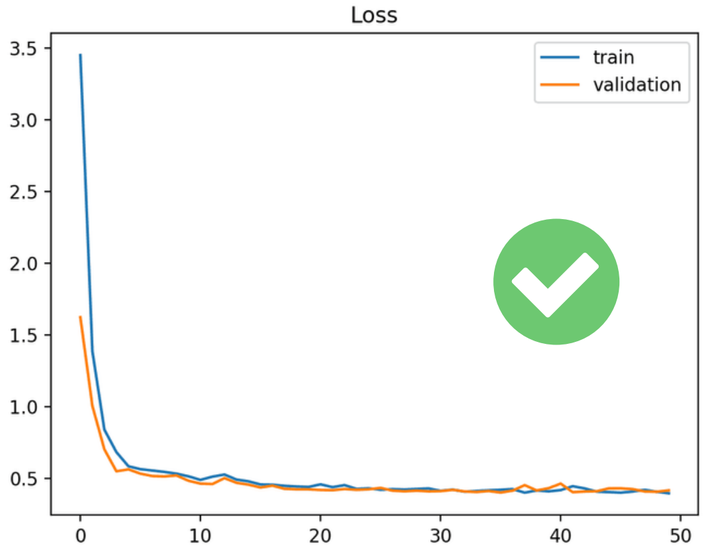


To describe the geomagnetic disturbances at mid-latitudes in terms of longitudinally asymmetric (ASY) and symmetric (SYM) disturbances for both H and D components respectively parallel and perpendicular to the dipole axis.
SYM-H is essentially the same as the Dst index with a different time resolution.

Siciliano et al, 2022

Diagnose

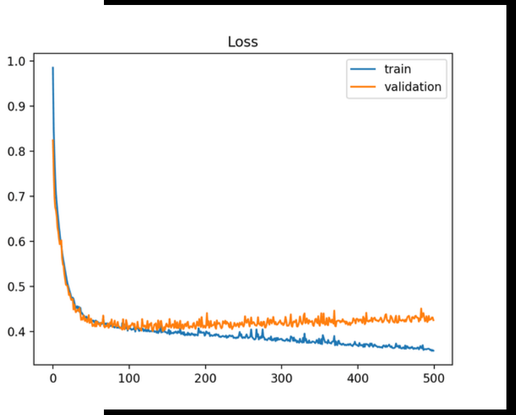
- The learning process



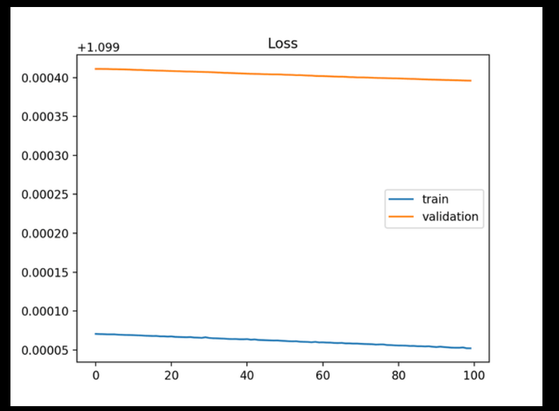
reallity

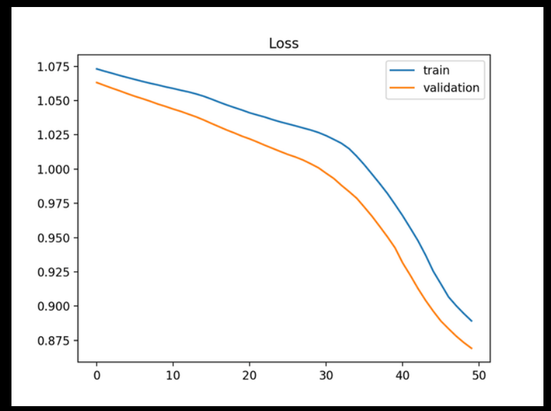
TSWC, 2022

overfitting



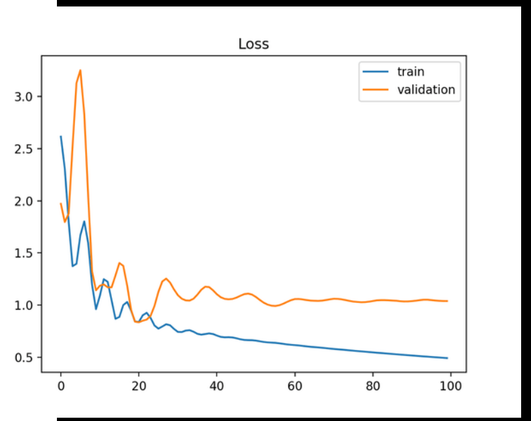
Model does not have a suitable capacity for the complexity of the dataset (underfit)





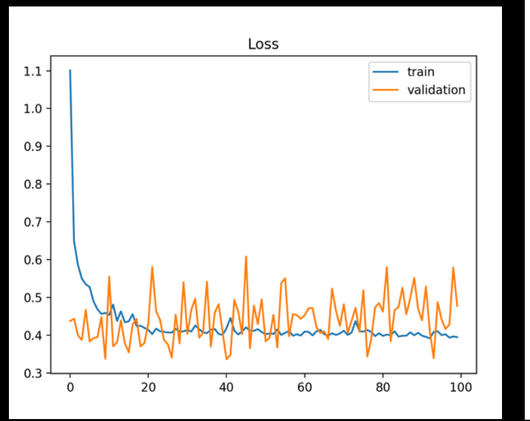
Model that requires further training (underfit)

unrepresentative training dataset

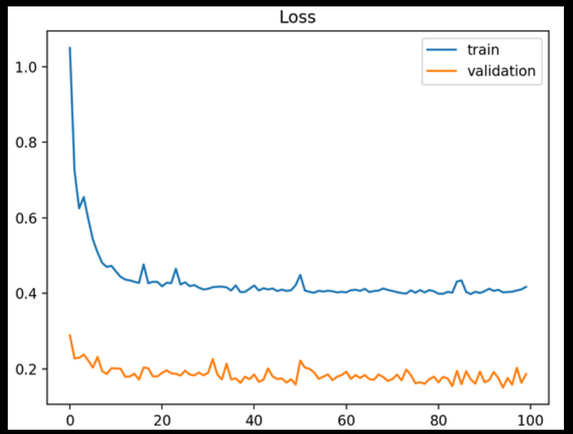


Dataset << relative to the validation dataset

unrepresentative validation dataset

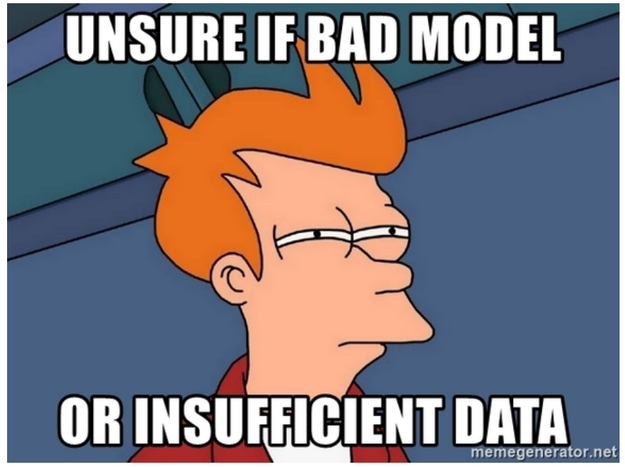


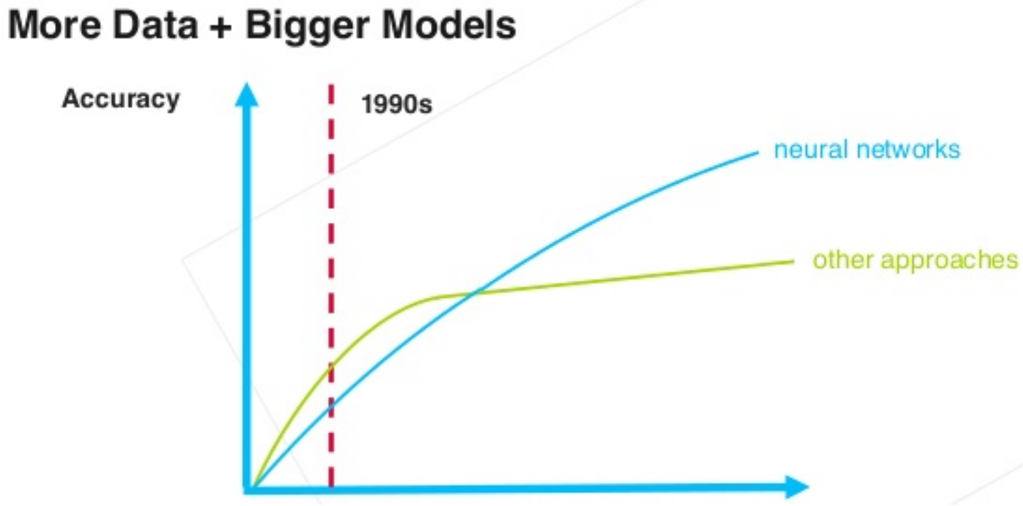
validation dataset does not provide sufficient information to evaluate the ability of the model to generalize

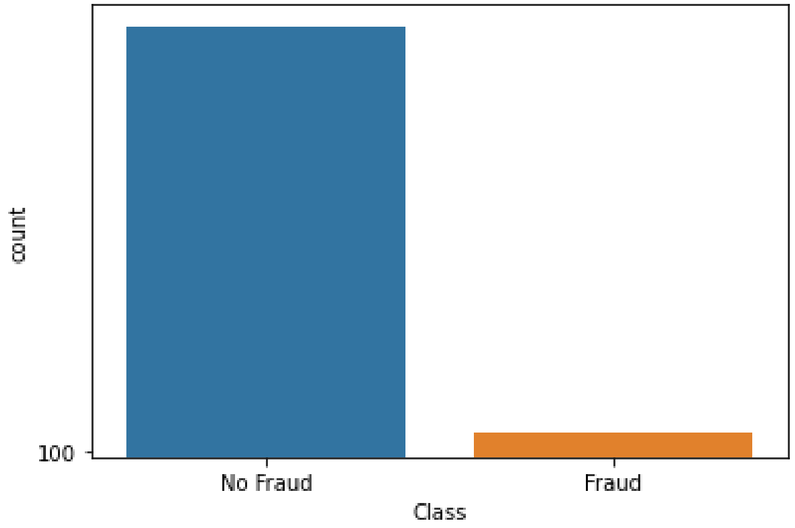


About the dataset

- Amount of data and data balancing





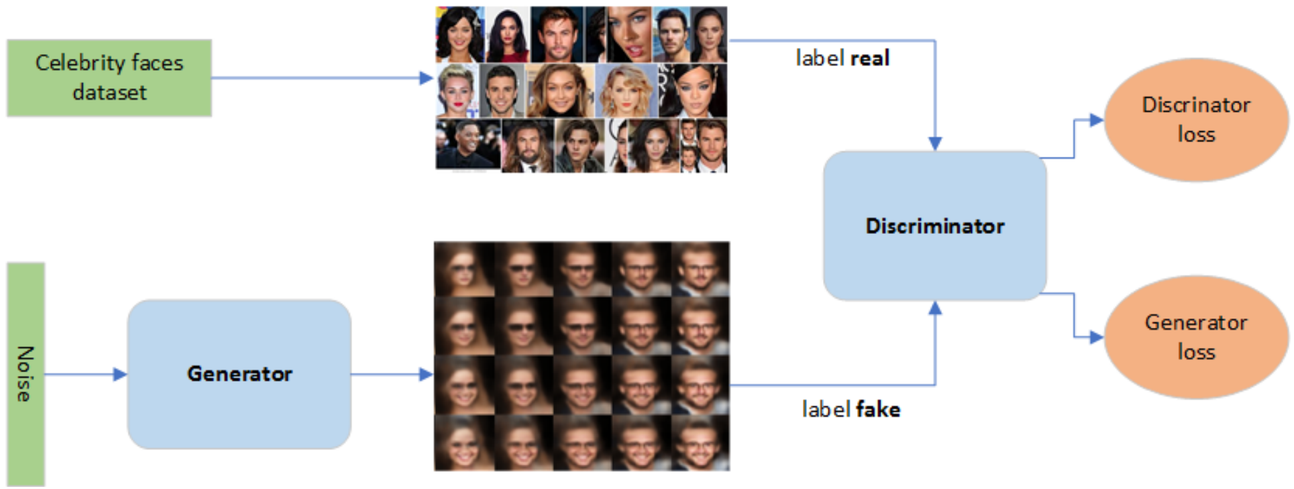


re sample (?)
generate more data (?)

About the dataset

Bertimas et.al., From Predictive Methods to Missing Data Imputation: An Optimization Approach (2018)

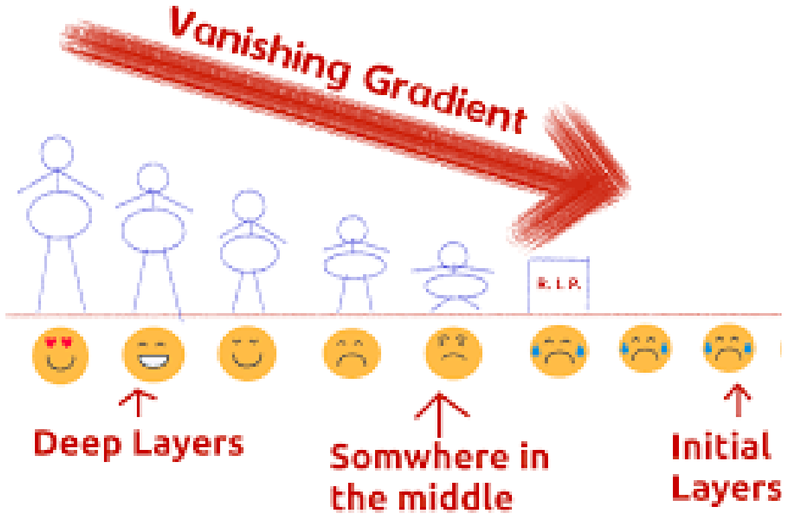
Method Name	Category	Software	Reference
Mean impute (`mean`)	Mean		Little and Rubin (1987)
Expectation-Maximization (`EM`)	EM		Dempster et al. (1977)
EM with Mixture of Gaussians and Multinomials	EM		Ghahramani and Jordan (1994)
EM with Bootstrapping	EM	`Amelia II`	Honaker et al. (2011)
K-Nearest Neighbors (`knn`)	K-NN	`impute`	Troyanskaya et al. (2001)
Sequential K-Nearest Neighbors	K-NN		Kim et al. (2004)
Iterative K-Nearest Neighbors	K-NN		Caruana (2001); Brás and Menezes (2007)
Support Vector Regression	SVR		Wang et al. (2006)
Predictive-Mean Matching (`pmm`)	LS	`MICE`	Buuren and Groothuis-Oudshoorn (2011)
Least Squares	LS		Bø et al. (2004)
Sequential Regression Multivariate Imputation	LS		Raghunathan et al. (2001)
Local-Least Squares	LS		Kim et al. (2005)
Sequential Local-Least Squares	LS		Zhang et al. (2008)
Iterative Local-Least Squares	LS		Cai et al. (2006)
Sequential Regression Trees	Tree	`MICE`	Burgette and Reiter (2010)
Sequential Random Forest	Tree	`missForest`	Stekhoven and Bühlmann (2012)
Singular Value Decomposition	SVD		Troyanskaya et al. (2001)
Bayesian Principal Component Analysis	SVD	`pcaMethods`	Oba et al. (2003); Mohamed et al. (2009)
Factor Analysis Model for Mixed Data	FA		Khan et al. (2010)



Goodfellow et.al. Generative Adversarial Networks (2014)

Vanishing gradient problem

- activation function, architecture, weight initialization, loss optimization algorithm, learning rate, ...



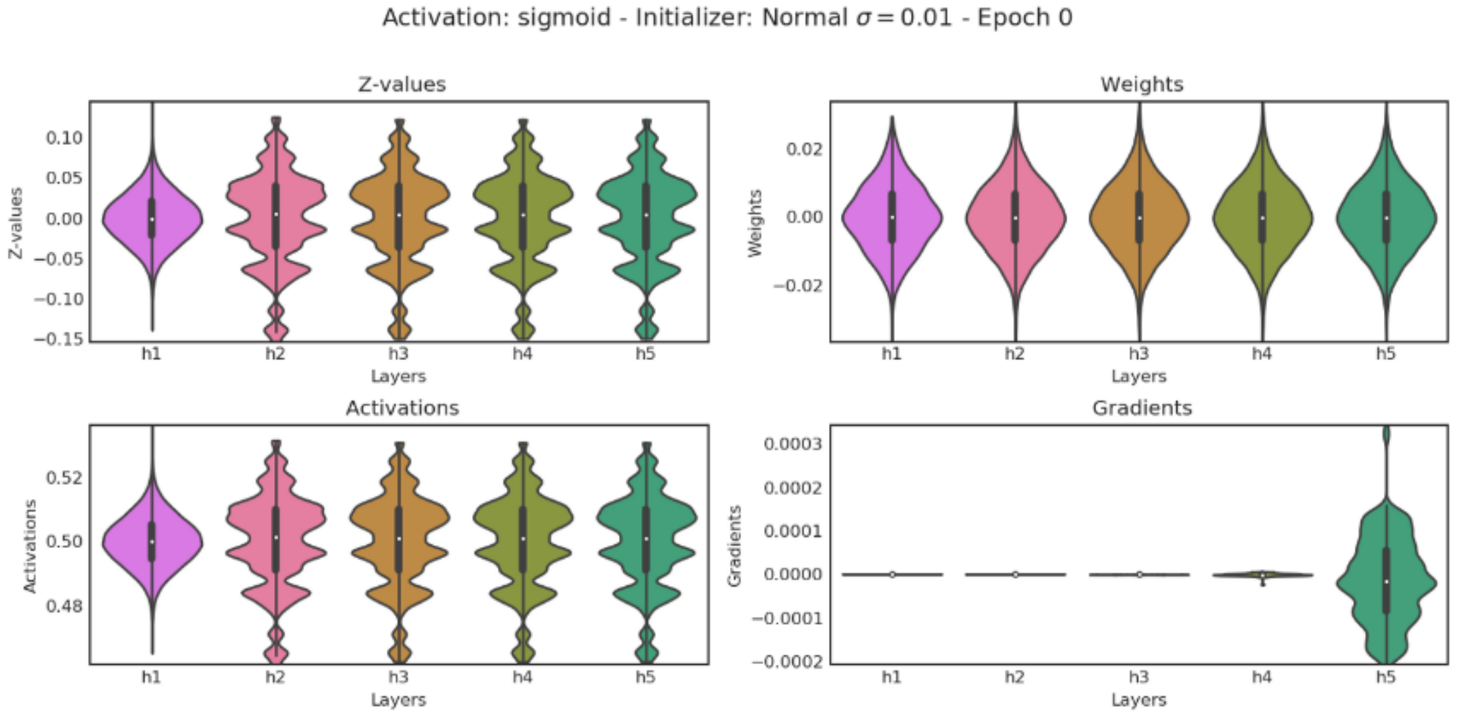


Figure 1. BLOCK model using sigmoid and naive initialization — don't try this at home!

https://towardsdatascience.com/hyper-parameters-in-action-part-ii-weight-initializers-35aee1a28404

Hyperparameters optimization

- Choose a set of optimal hyperparameters for a learning algorithm (maximizes the model performance)
- Hyperparameters are set before the learning process (#neurons, #cells, loss optimization algorithms, etc)

GRID SEARCH

1 —Identify the model's hyperparameters to optimizest.

2 — Asses error score for each combination in the hyperparameter grid.

3 — Select the hyperparameter combination with the best error metric.

Hyperparameters optimization

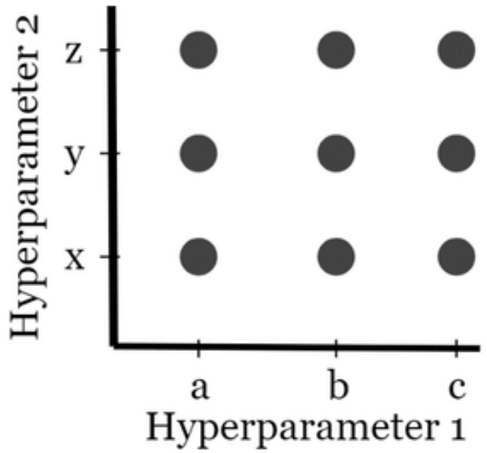
```
# learning_rate choices
 learning_rates = [ 0.1, 0.2, 0.3, 0.4, 0.5,
                    0.01, 0.02, 0.03, 0.04, 0.05 ]
 # iterations choices
 iterations = [ 100, 200, 300, 400, 500 ]

 parameters = []
 for i in learning_rates :
     for j in iterations :
         parameters.append( ( i, j ) )

 print("Available combinations : ",  parameters )

 # Applying linear searching in list of available combination
 # to achieved maximum accuracy on CV set

 for k in range( len( parameters ) ) :
   #  model = METHOD(..., learning_rate = parameters[k][0],iterations = parameters[k][1] )
   # ...
```

Hyperparameters optimization

Grid Search

Pseudocode

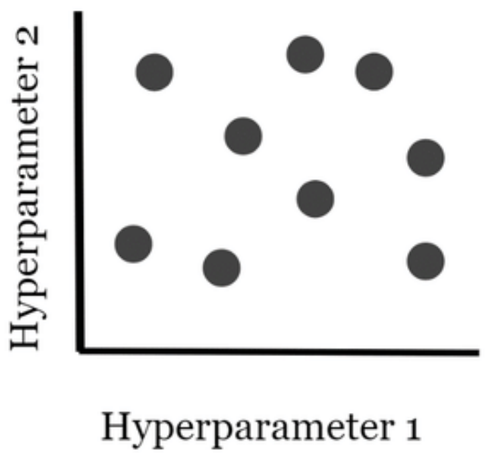
```
Hyperparameter_One = [a, b, c]
Hyperparameter_Two = [x, y, z]
```



Random Search

Pseudocode

```
Hyperparameter_One = random.num(range)
Hyperparameter_Two = random.num(range)
```

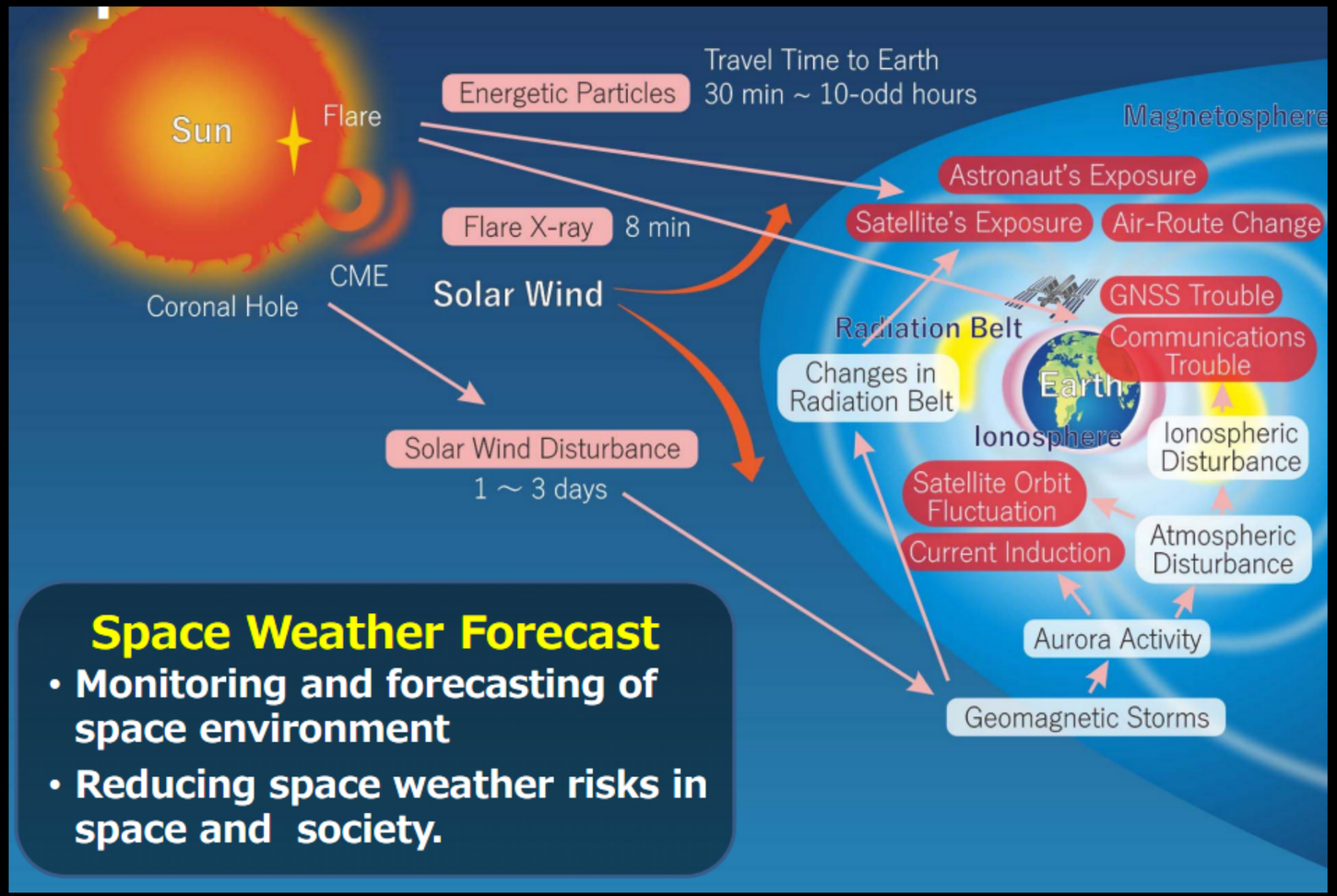


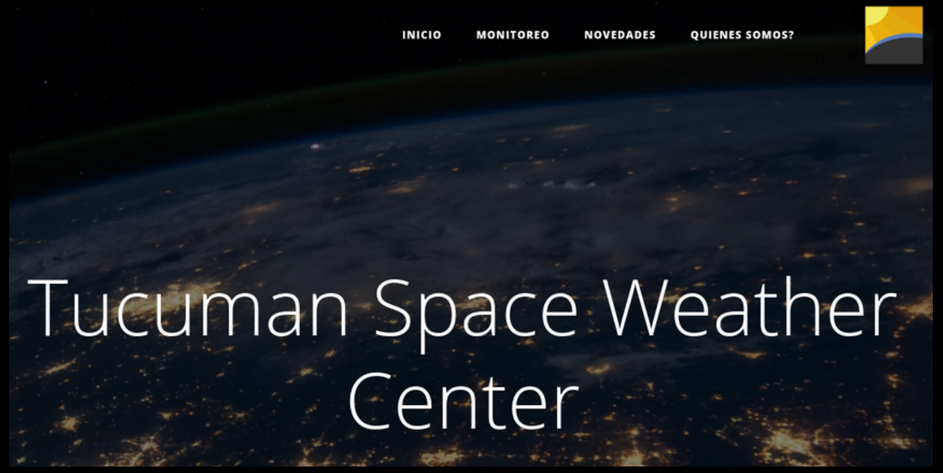
Other methods

- Bayesian Optimization
- Evolutionary Optimization.

https://towardsdatascience.com/hyperparameters-tuning-from-grid-search-to-optimization-a09853e4e9b8

Something we are working on ...





https://spaceweather.facet.unt.edu.ar/
Instagram: /spaceweatherargentina

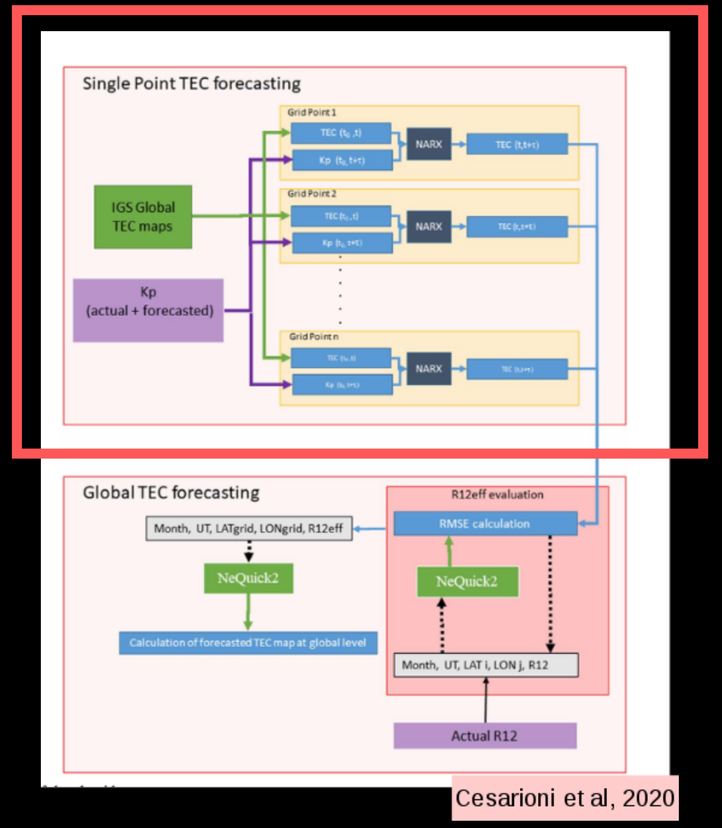
The problem: 24hs forecasting of TEC given information regarding geomagnetic conditions

GLOBAL TEC FORECASTING

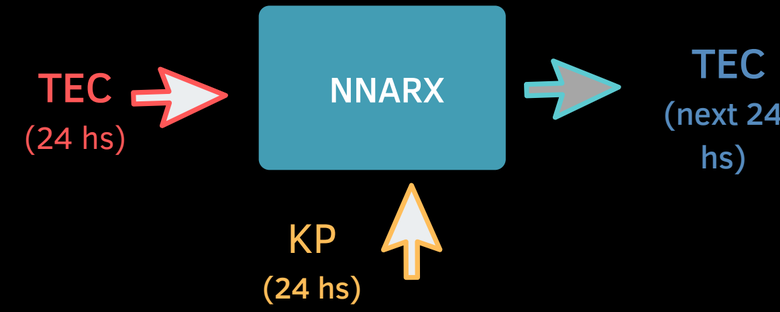
In prep

TSWC, 2022

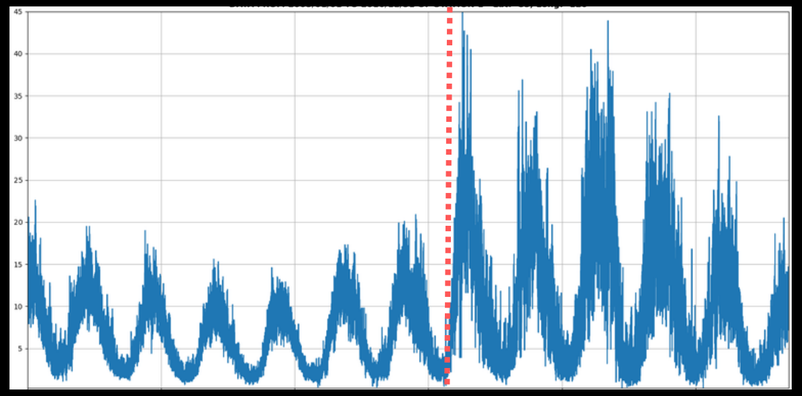
- 24 hs ahead
- Dataset: 2005 - 2016
- **Input**: Global Ionospheric Map (GIM) from IGS. Spatial-temporal res 2.5° (lat) - 5° (lon) - 2 h
- **External forcing** (* SWx): Kp index
- Loosely physics-informed ML

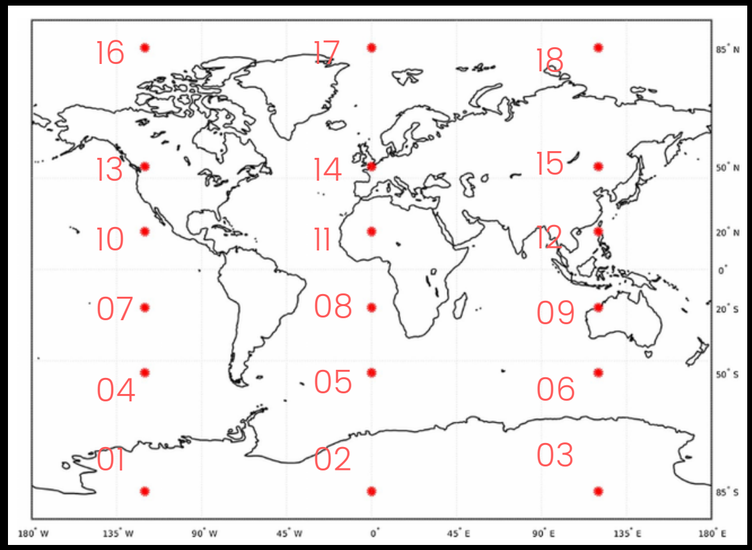


Cesarioni et al, 2020



St 01 - dataset (2005 - 2016)



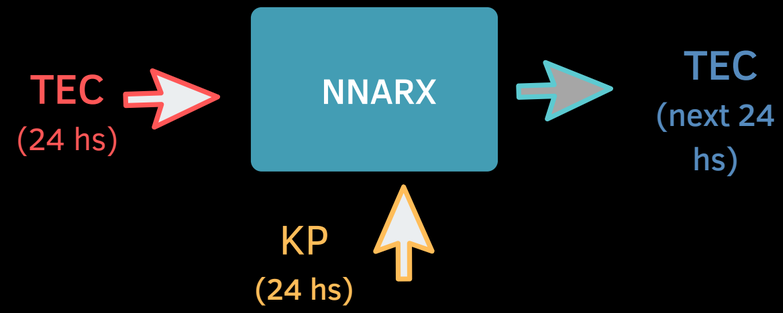


(Molina et al, ESWW 2021)

GLOBAL TEC FORECASTING

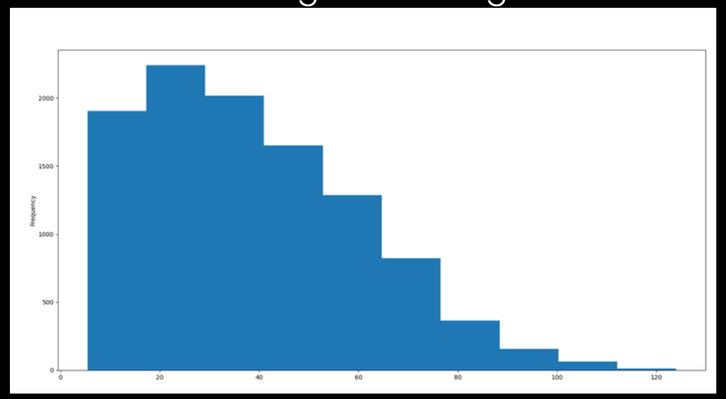
In prep

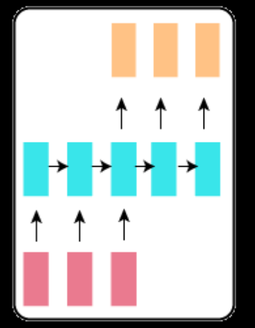
TSWC, 2022



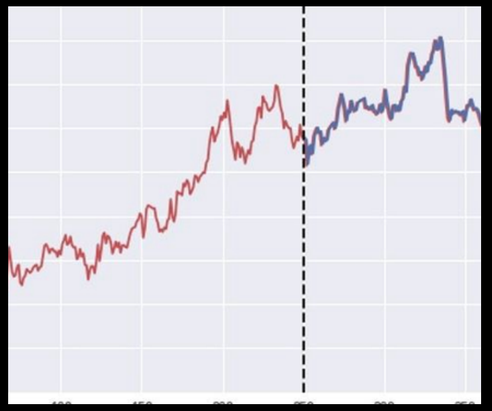
- Train: 99 %(99/1) Test: 1 %
- Re-sampling:
  - GIM 2 hs resolution
  - Kp 3hs resolution > K Nearest-neighbor interpolation
- No missing values
- Kernel initializer: GlorotNormal distribution

TEC - single ST Histogram





- DL modeling
  - 24 hs (before) to forecast 24 hs (ahead) - 24 hs = 12 samples
  - supervised ML
  - 3 methods
  - time-series

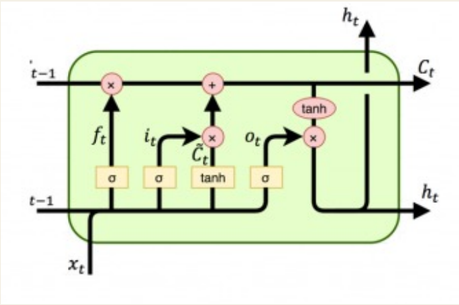


(Molina et al, ESWW 2021)

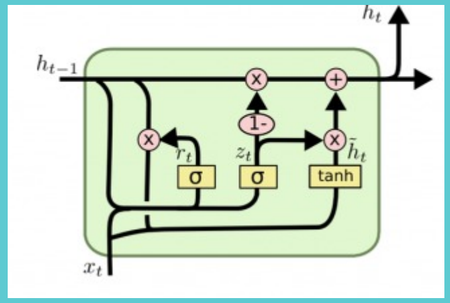
GLOBAL TEC FORECASTING

TSWC, 2022

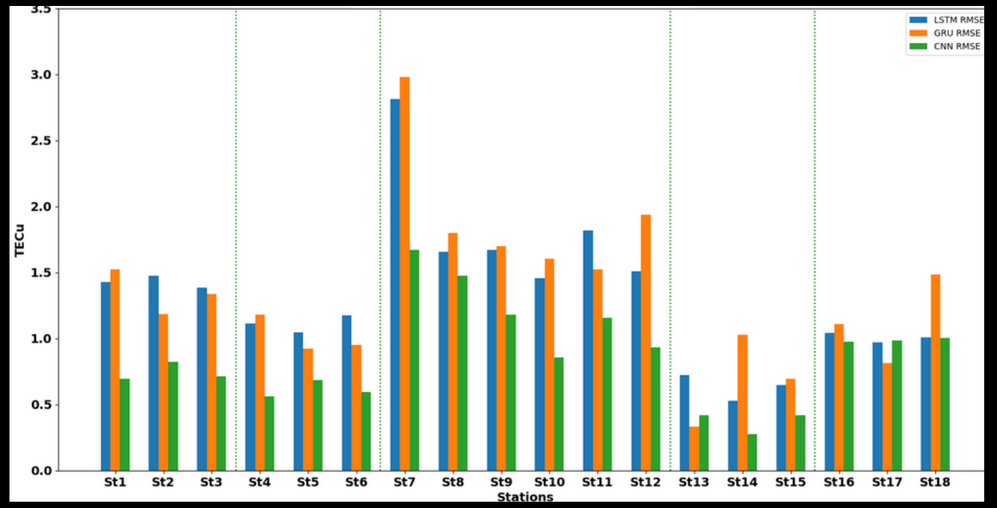
LSTM



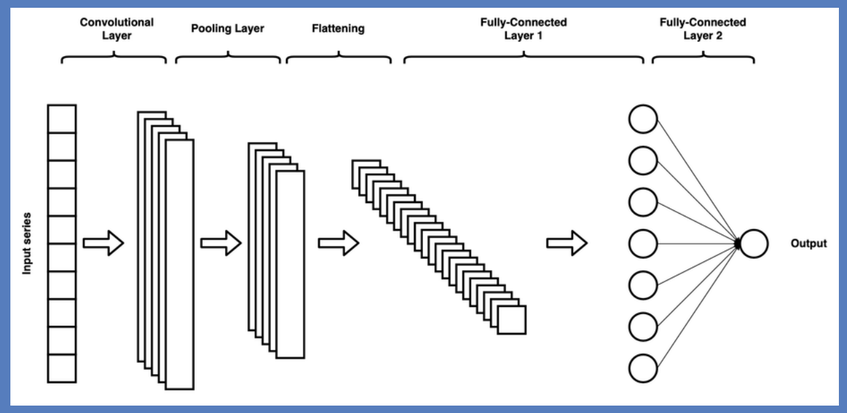
GRU

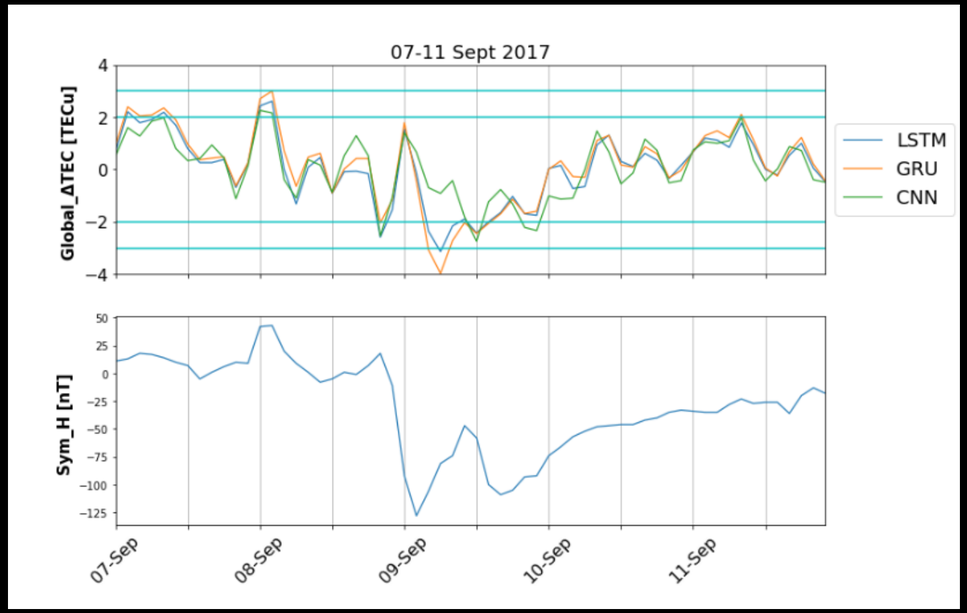


(Molina et al, ESWW 2021)



CNN - 1D



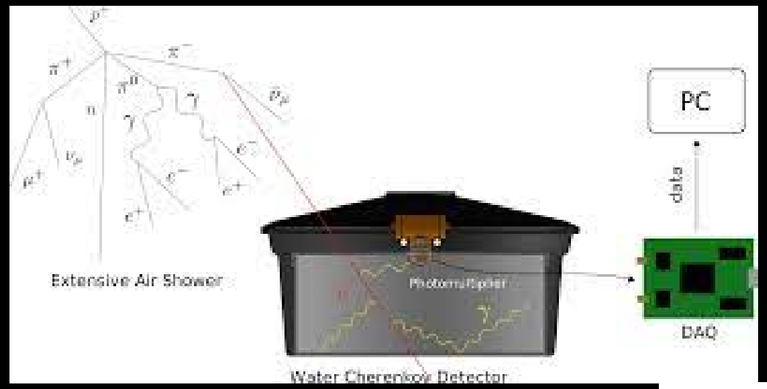


In prep

Ticiano Torres Peralta

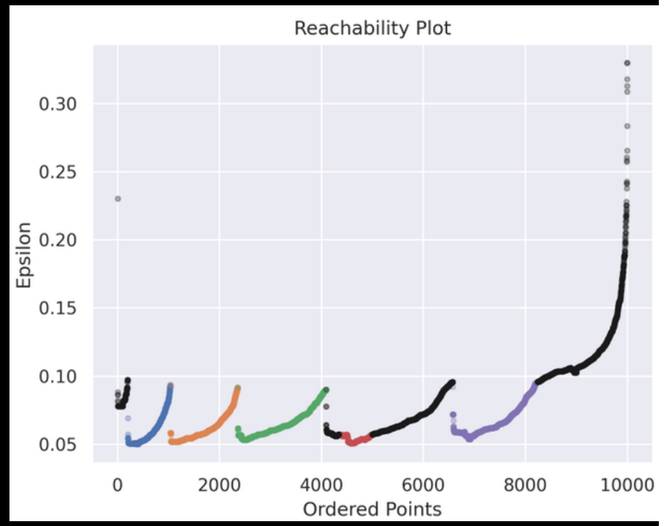
Something (else) we are working on ...

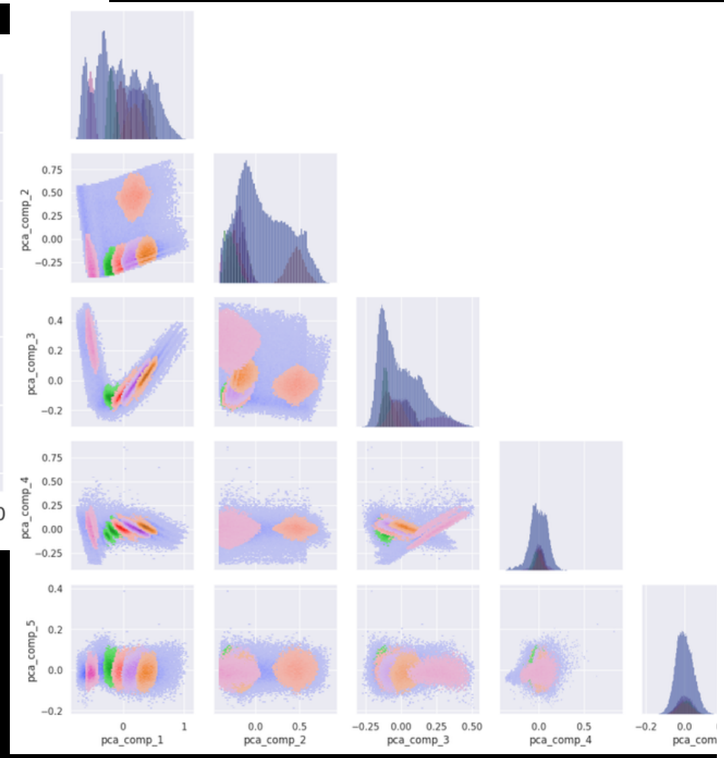
Clustering: Ordering points to identify the clustering structure (OPTICS)

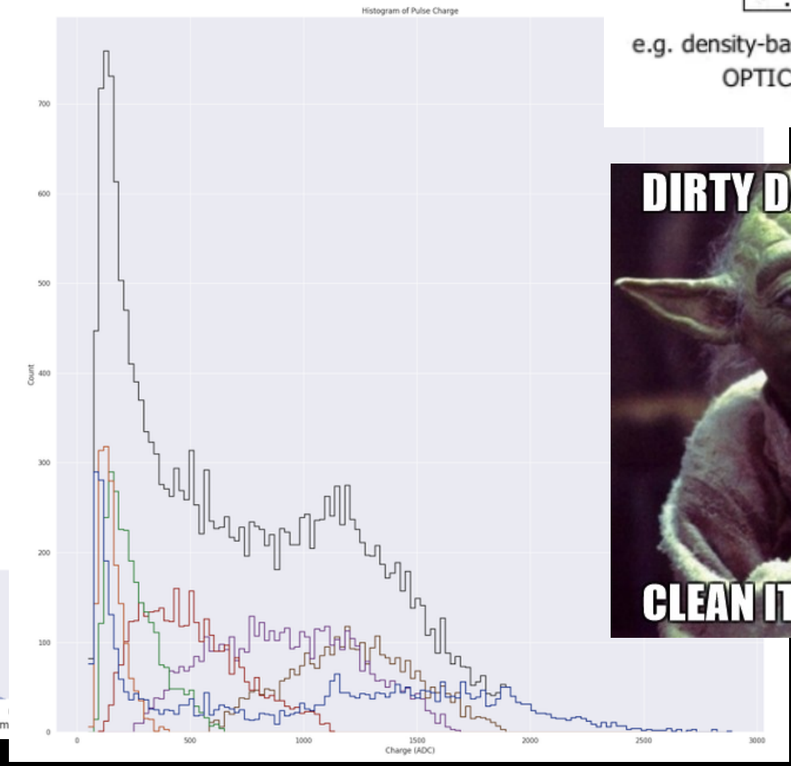


http://lagoproject.net/

In prep

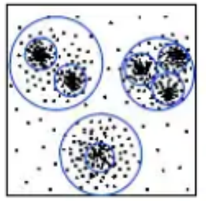






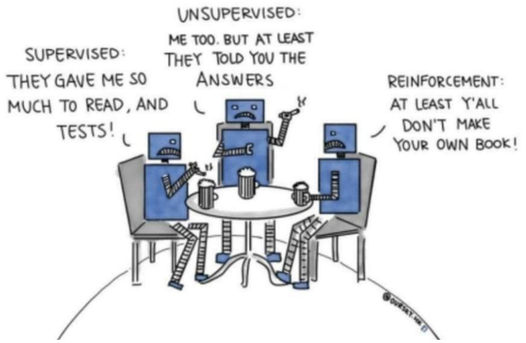
Hierarchical Clustering

nested clusters

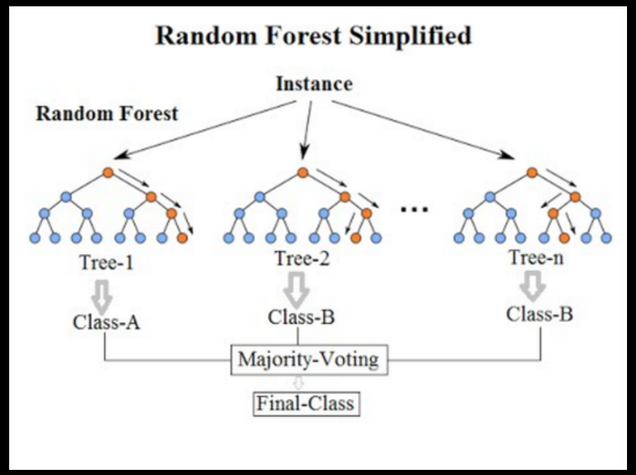


e.g. density-based clustering algorithm
OPTICS [SIGMOD 99]

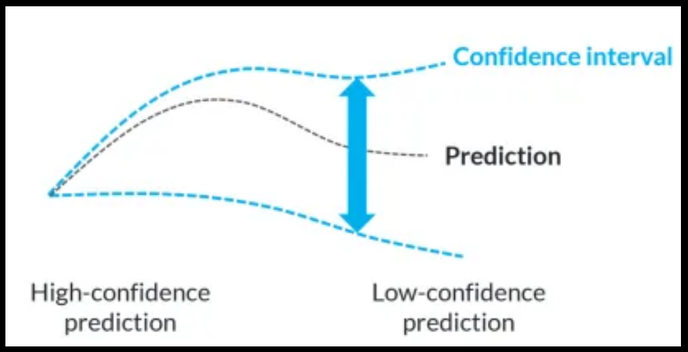
MACHINE LEARNING



- Ensemble techniques

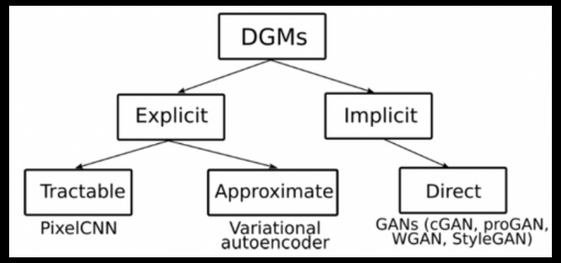


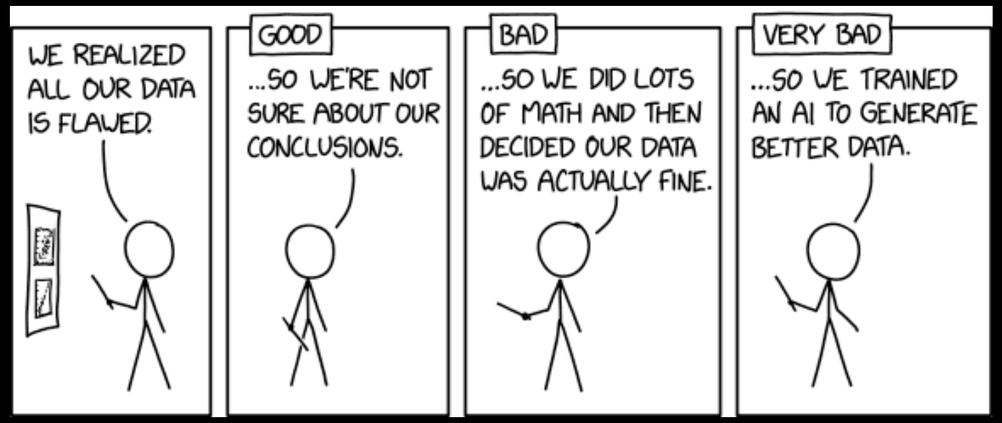
- Uncertanty Quantification (BNNs) - trustworthiness

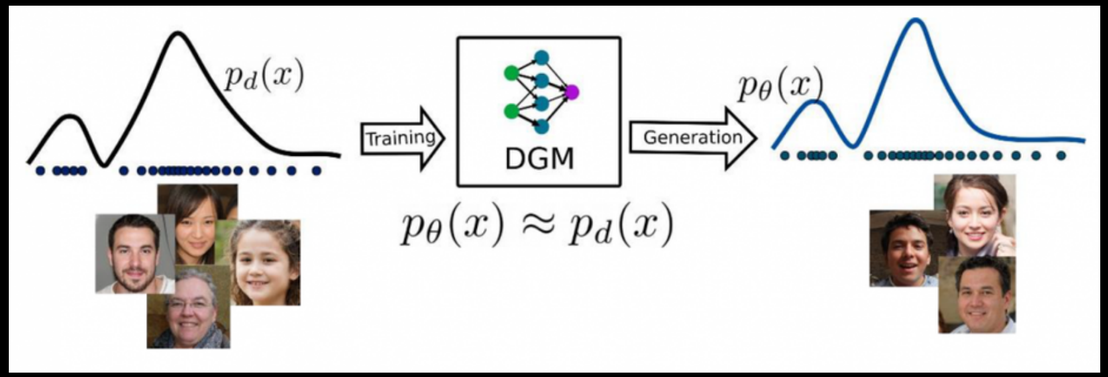


- Transformers
- Transfer Learning !

- Deep Generative Models







- (ML in production) Real -time -> re-training, incremental training, etc

and much more!!!

OPEN DISCUSSION

International Workshop on Machine Learning for Space Weather: Fundamentals, Tools and Future Prospects

7-11 November 2022
This is a hybrid meeting
Buenos Aires, Argentina

Further information:
https://indico.ictp.it/event/9840/
smr3750@ictp.it
+39-040-2240284
Elizabeth Brancaccio

Dra María Graciela Molina
FACET-UNT / CONICET
Tucumán Space Weather Center - TSWC

https://spaceweather.facet.unt.edu.ar/
IG -> @spaceweatherargentina

gmolina@herrera.unt.edu.ar