

Applications of computer vision and forecasting to the CERN accelerators

F. M. Velotti, B. Goddard, V. Kain with many inputs from ML community forum

Outline



- → Introduction
- → CNN for beam dump system analysis
 - ♦ Brief intro to CNNs and AE
 - VAEs for beam dump screen analysis
- → LSTMs for kicker temperature predictions
 - Brief intro to LSTMs
 - Application of LSTMs models to kicker temperature prediction
- → Physics Informed Neural Networks
 - Brief intro to PINN
 - ◆ Application of PINN to hysteresis predictions
 - Simple example of PINN
- → Summary



→ How do we use Convolutional Neural Networks (CNN)?



→ How do we use Convolutional Neural Networks (CNN)? Obviously, to recognise a cat! []]



→ How do we apply time-series forecasting?



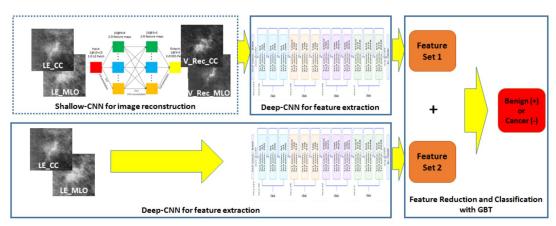
→ How do we apply time-series forecasting? Obviously, to predict stock market!



Introduction (serius now)



- → Huge achievements in image analysis with Convolutional Neural Networks (CNN)
 - Cancer tumores diagnostic from images (e.g. [2], [3]): in use in many institutes



Skin Cancer detection using ABCD rule and TDS value Classification of Skin Cancer using CNN

Fig. 3. Architecture of Shallow-Deep CNN



- → Huge achievements in image analysis with Convolutional Neural Networks (CNN)
 - ◆ Cancer tumores diagnostic from images (e.g. [2], [3]): in use in many institutes
 - Here is a guide how to make a style changer app

























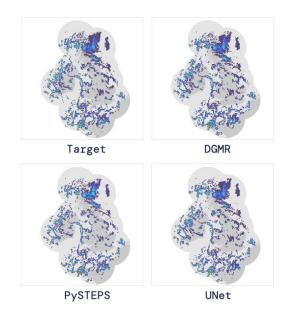






- → Time-series prediction is another extremely active research topic
- → Weather nowcast is a perfect example of how the 2 model types can work together [4]







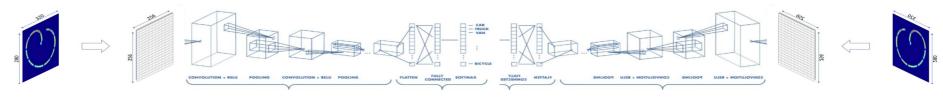
CNN for beam dump system analysis

Example of CNNs @ CERN accelerators



- → SPS and LHC beam dump systems:
 - ♦ BTV just before absorber block => image of the dumped beam
- → GOAL: infer the state of the dump system from image and extract anomalous system

Physical system: $C[k_v,k_h, au,...]$ Input: X[m,n] Output: $ar{C},ar{X}$



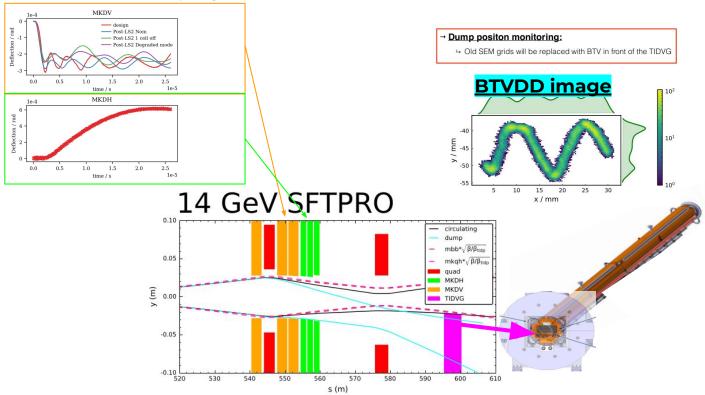
Feature extraction

Regression

Just a little step back: SBDS



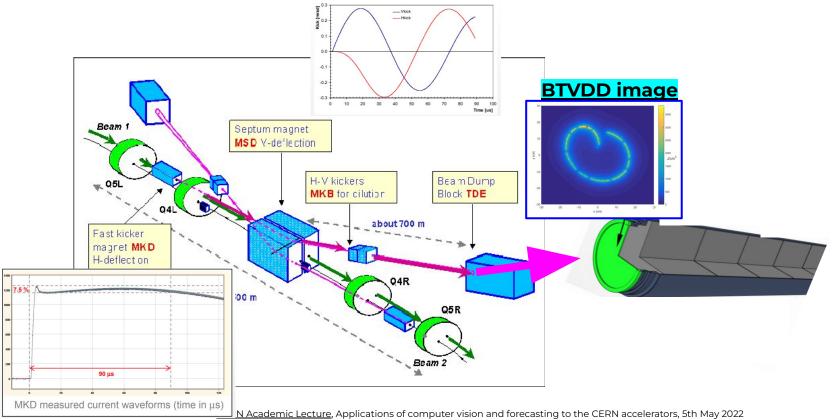
→ The SPS dump system in a nutshell



Just a little step back: LBDS



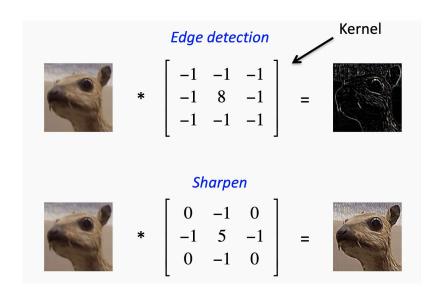
→ The LHC beam dump system in a nutshell

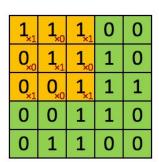


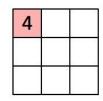
Convolutional NN



- → CNN are neural networks that are mainly used for image processing
- → We can see it as a sliding filter on the image







Image

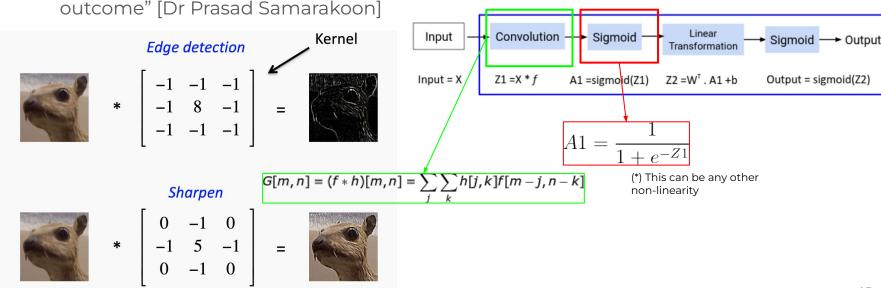
Convolved Feature

Convolutional NN



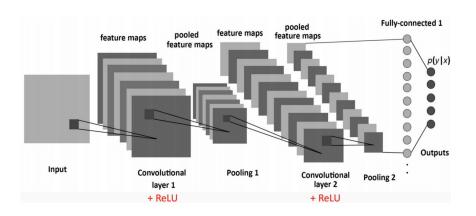
- → CNN are neural networks that are mainly used for image processing
- → We can see it as a sliding filter on the image => not a black box but just a complicated function on many dimensions!

• "Looking at the a function's surroundings to make better/accurate predictions of its



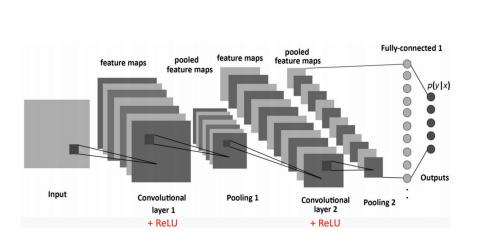


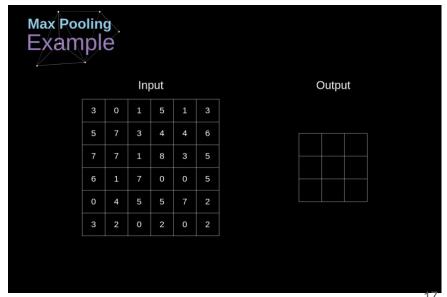
→ CNN models are a sequence of CNN layers, but not only...





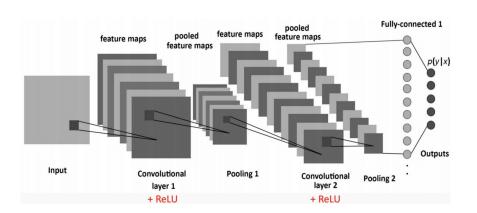
- → CNN models are a sequence of CNN layers, but not only...
 - Max pooling

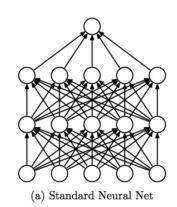


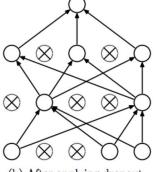




- → CNN models are a sequence of CNN layers, but not only...
 - Max pooling, dropout



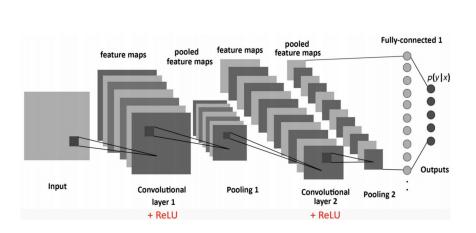


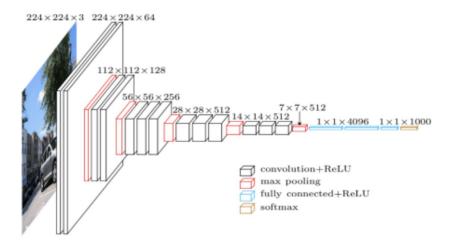


(b) After applying dropout.



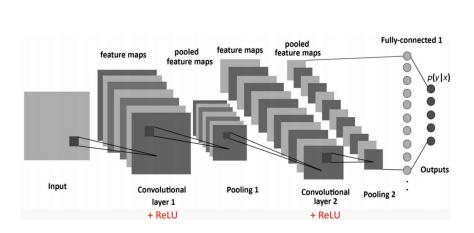
- → CNN models are a sequence of CNN layers, but not only...
 - Max pooling, dropout, linear layers...
 - ♦ They can be used for classification or regression

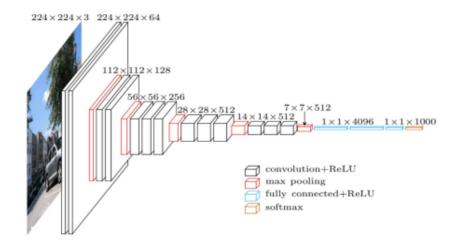






- → CNN models are a sequence of CNN layers, but not only...
 - Max pooling, dropout, linear layers...
 - ♦ They can be used for classification or regression
 - Very clear explanation how CNN work <u>here</u>

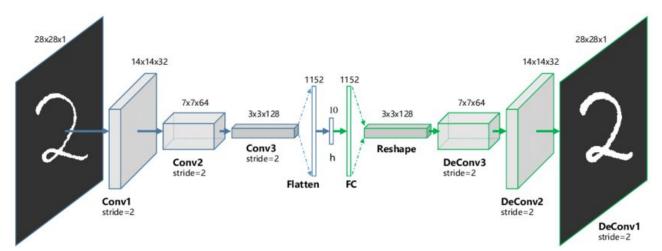




Auto Encoders and Variational AE



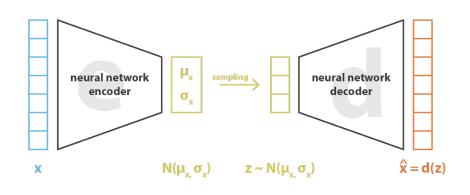
- → Auto Encoders are just a type of NN that aims to learn efficient encoding of the unlabelled data (unsupervised learning)
 - ◆ This is done regenerating the input parameters (images, vectors, scalars), e.i. minimising the reconstruction error of the input
- → Usually used for dimensionality reduction (kind of non-linear PCA), denoising, generative models, translation...



Auto Encoders and Variational AE



- → Variational Auto Encoders (VAE) [12] are special type of encoder
 - Express the latent attributes as probability distribution
- → This leads to smooth latent state representation of the input => towards generative interpolating models



loss =
$$||x - x^2||^2 + KL[N(\mu_v, \sigma_v), N(0, I)] = ||x - d(z)||^2 + KL[N(\mu_v, \sigma_v), N(0, I)]$$

Kullback-Leibler Divergence

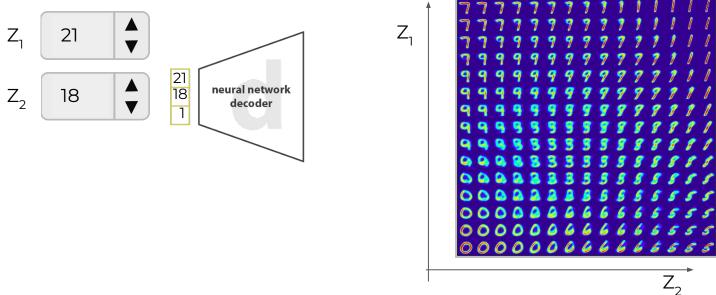
$$D_{KL}(p||q) = \sum_{i=1}^N p(x_i) \cdot log rac{p(x_i)}{q(x_i)}$$



Auto Encoders and Variational AE



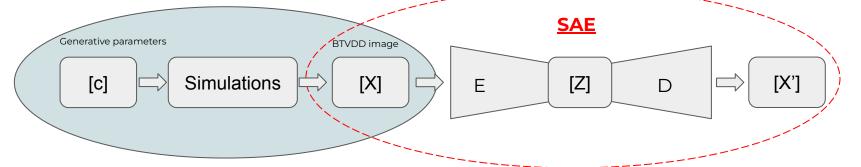
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VAE for BTVD image reconstruction

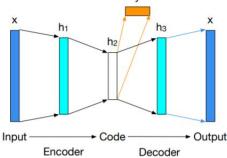


→ Special case of VAE => Supervised [Variational] Auto Encoder (idea taken from [5])



$$L_{i}(\theta,\phi) = -E_{z \sim q\theta(z|x_{i})}[\log_{\phi}(x_{i}|z)] + \mathbf{w}_{KL} KL(q\theta(z|x_{i}), p(z)) + \mathbf{w}_{g} MSE(\mathbf{c}, \mathbf{Z})$$

_- !=0



VAE for BTVD image reconstruction



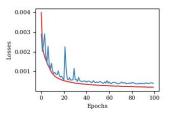
- → All the snippet prested developed in <u>Pytorch</u>
- → Started from the VAE [6]
- → Many modification to the model were made to make it tunable at need
 - Our model is available [7] for the LBDS and very similar for SBDS
 - Custom loss function

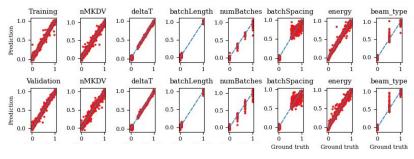
```
"Reconstruction Loss": recons loss,
```

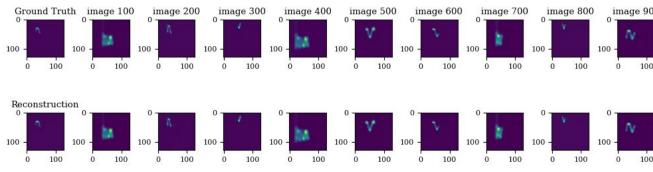
BTVDD image reconstruction in SPS



- → Very accurate prediction from simulations
- → Batch spacing reconstruction not obvious (very difficult to see)
- → Reconstructed images almost indistinguishable



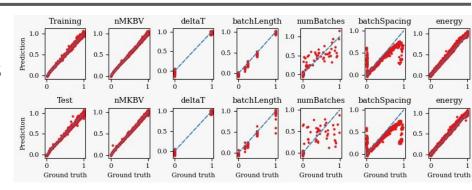


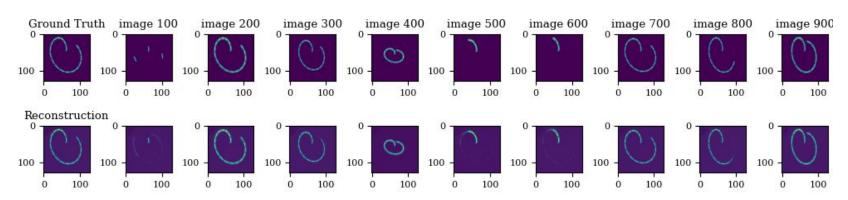


BTVDD image reconstruction in LHC



- → Similar results for LHC
- → Here the most complicated part is to simulate different filling patterns
 - Number for batches very difficult for many single bunches
 - batch spacing very difficult for single bunches

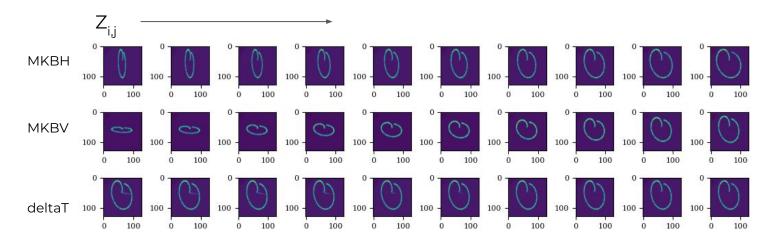




Latent space scan



- → With this architecture, we can generate BTVDD images from generative parameters (number of kickers...) using the decoder by itself
- → Orthogonal scan possible

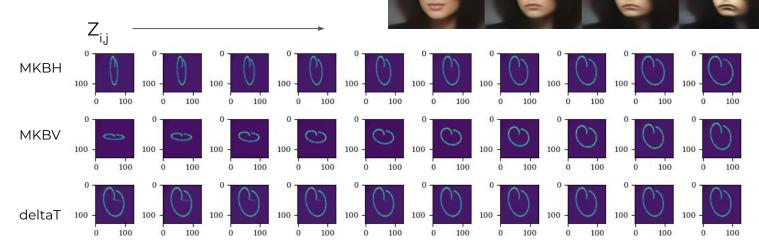


Latent space scan



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Deploy on real data

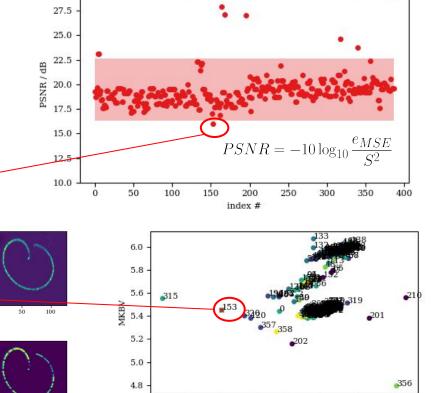
50



4.2

30

- → Of course the final goal is to predict real images...
- → Using both generative parameters and image reconstruction score, anomalous case found!



3.5

3.6

3.9

MKBH

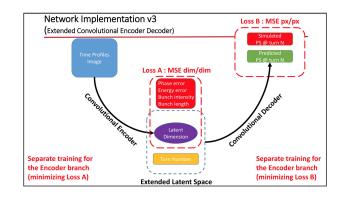
4.0

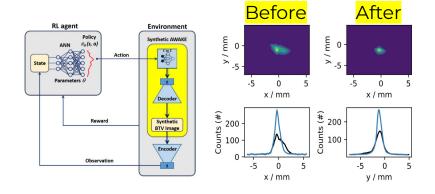
30.0

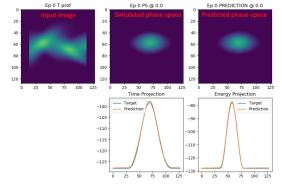
Other examples



- → Neural Longitudinal tomography in the LHC
 - Classically limited to single bunch => with ML no limits!
- → Unsupervised stated encoding for RL applied on AWAKE transfer line matching agent
 - Use of the encoded information of BTV image to match beam size to requested one







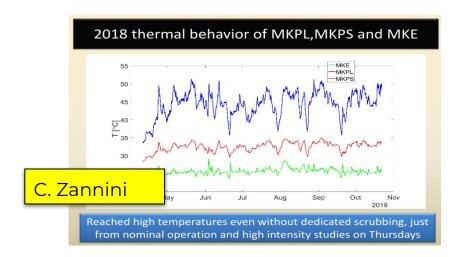


LSTMs for kicker temperature predictions

Introduction to the problem



- → The MKP-L is one of the main limiting element for high intensity
 - Beam induced heating is directly related to the beam power loss through the real part of the longitudinal impedance
- → Temperature observed to be much higher than normal operation also during 2018's HI MDs



Model for the MKP-L heating evolution

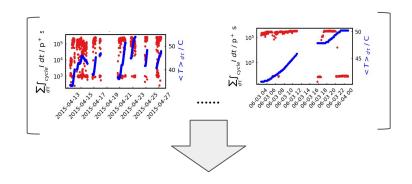


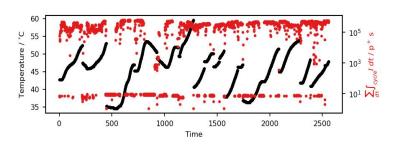
→ Neural networks to <u>estimate the</u> <u>temperature evolution of the MKP</u> <u>as a function of the intensity and</u> <u>history</u>

- Should be able to suggest the best strategy to optimise scrubbing
- ♦ Keep MKP temperature below limits
- Reduce idle time

→ This is a time series!!

- LSTMs are a very good choice for these kind of problems
- → <u>Input data:</u> Intensity integrated over 5 min, bunch length, peak intensity and temperature history

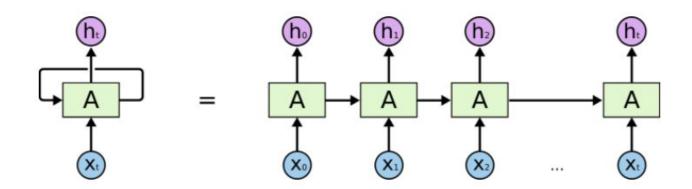




Recurrent Neural Networks



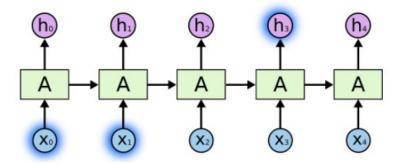
- → DNN (as seen in one of the first lectures) cannot "remember" previous estimations as they deal with instantaneous data
- → Recurrent NN (RNN) address this issue (source [6])
 - ◆ The input is passed to the same NN and the output is then recursively injected in the following prediction



Recurrent Neural Networks



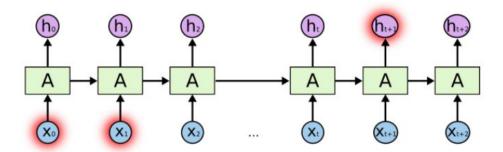
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Recurrent Neural Networks

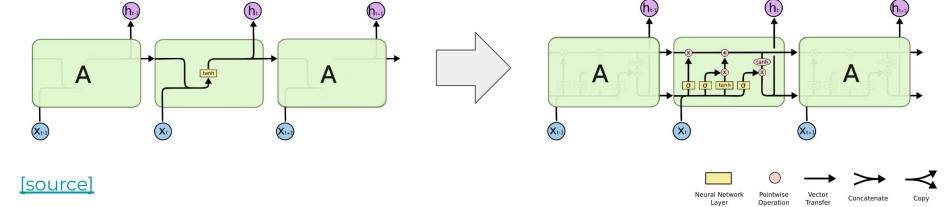


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- → Recurrent NN (RNN) address this issue (source [6])
 - The input is passed to the same NN and the output is then recursively injected in the following prediction
- → It works great for "recent" predictions
- → But it struggles for information further back in time [7]



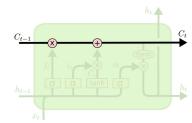


- → In rescue of the RNN and their exploding/vanishing gradient issues (see [7] for more details) come the LSTMs
- → Capable of "remembering" information for long sequences
- → Intuition:
 - Select important part of sequence to remember



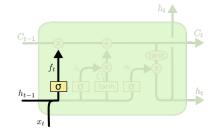


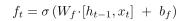
→ Information flows via cell state from one time stamp to another (with some linear interaction with other gates)

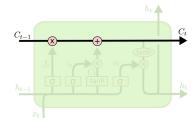




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- → The "forget gate" decides how much of the cell state C_{t-1} we keep

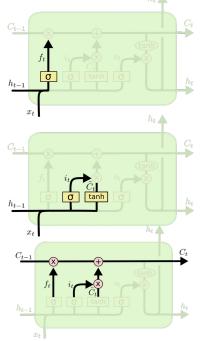




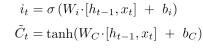


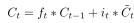


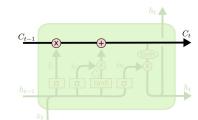
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- → The input gate processes the input and proposes a new C₊



$$f_t = \sigma \left(W_f \cdot [h_{t-1}, x_t] + b_f \right)$$

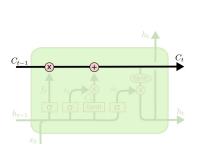


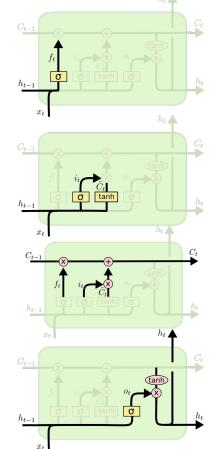






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- → Finally, we output h_t for the next cell or to be used as it is





$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)$$

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

$$o_t = \sigma (W_o [h_{t-1}, x_t] + b_o)$$

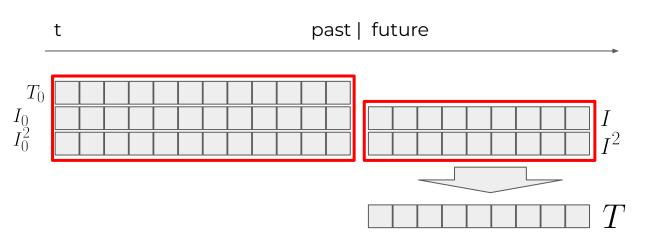
$$h_t = o_t * \tanh (C_t)$$



LSTM model for MKP temperature



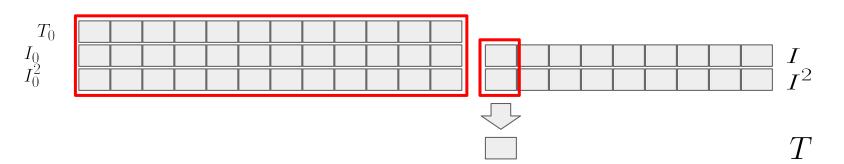
- → Very simple architecture: basically one LSTM layer and a dropout layer before a linear one
- → Add known future input (main difference wrt classic time-series prediction models)



```
class LSTM_FB(nn.Module)
 def __init__(
    self.
   rnn num layers=1.
    input_feature_len=2,
    sequence len=35.
    hidden dim=100.
   max output size=30
    device="cpu".
    dropout=0.2.
    super().__init__()
    self.sequence len = sequence len
    self.hidden dim = hidden dim
    self.input feature len = input feature len
    self.num layers = rnn num layers
    self.lstm = nn.LSTM(
      num_layers=rnn_num_layers,
      input_size=input_feature_len,
      hidden size=hidden dim.
      batch first=True
      dropout=dropout.
    self.max output size = max output size
    self.out layer = nn.Linear(self.hidden dim, 1)
    self.device = device
```

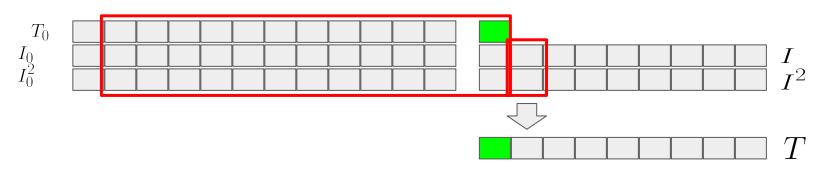


- → Our idea: iterative prediction => teacher forcing for all samples
 - Losses calculated on a fixed sequence length and not value by value
- → Advantages:
 - NN already exposed to its noise in the training phase already
 - ◆ The output sequence is obtained in one call of the NN (see later for the implementation)
 - Arbitrary output length



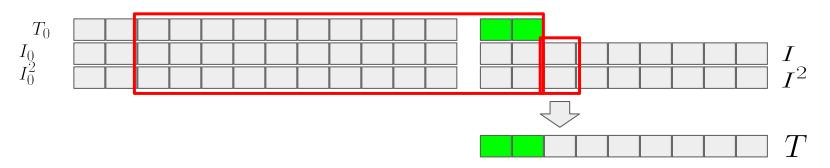


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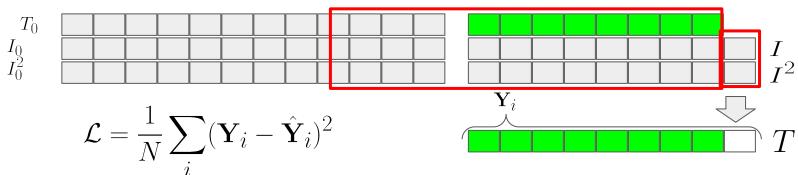


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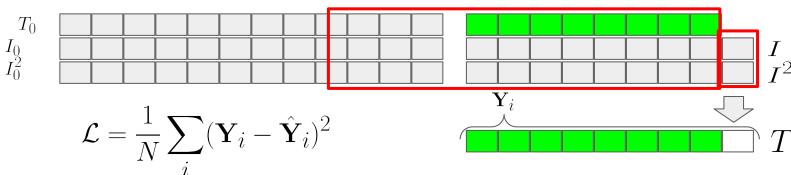
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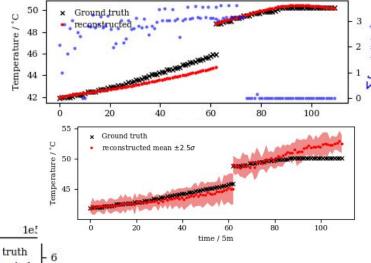
Then backpropagation step using this predicted sequence

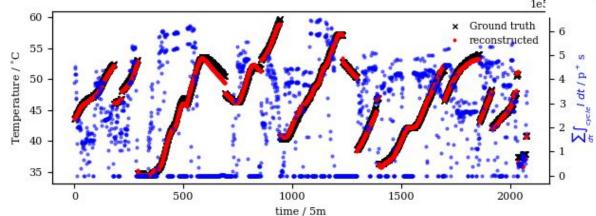


LSTM model for MKP: results



- → Trained model repreduced training and validation data set almost perfectly
 - Error in the order of a couple of degrees on test dataset
- → Bayesian version looking also promising

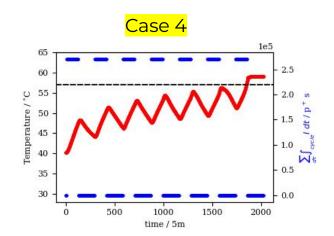


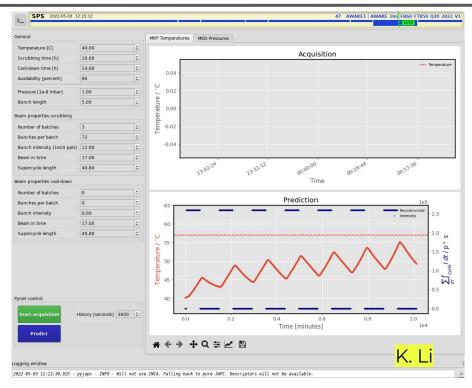


Summary and prediction



- → Testing prediction on different scenarios
- → Summary:
 - Model results very promising
 - Model ready and used in CCC to make estimation of time left for HI beams
 - Model not capable to extrapolate
- Need to include physics in the model...

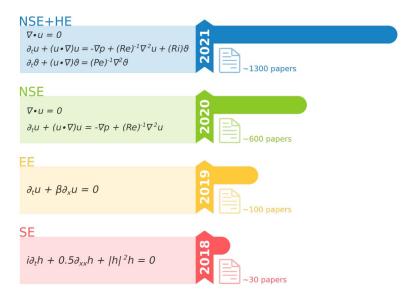






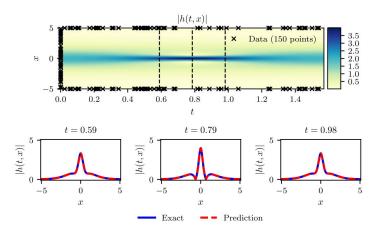


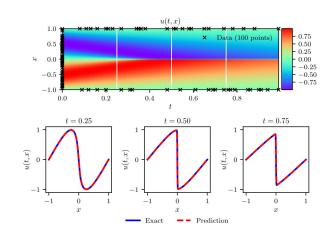
- → Embedding physics knowledge in NN is becoming very common
- → Very complete summary of applications [11] (figure taken from [11])





- → First proposed to solve nonlinear PDE [10] (all plots from [10])
- → Basically using boundary and initial conditions values, NN can interpolate the whole system dynamics "knowing" the PDE that describe the system
 - ◆ At the same time though, one can just use a physics loss term...it doesn't have to be a PDE system (IMO)

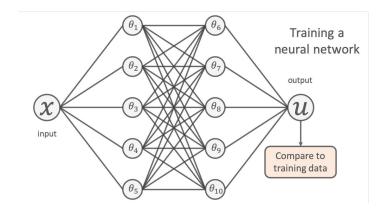




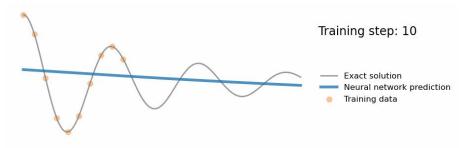


→ DNN cannot extrapolate beyond the training domain...which is exactly what we would expect from interpolation function

$$min(Loss) => Loss = Mean(data - prediction)^2$$



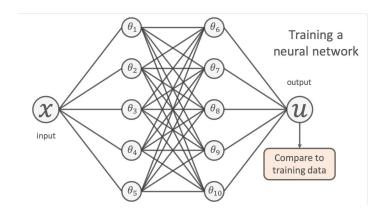
Source: [8]



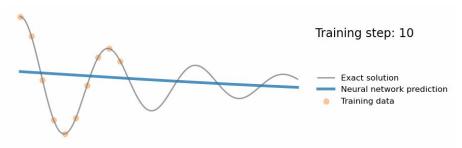


→ DNN cannot extrapolate beyond the training domain...which is exactly what we would expect from interpolation function

$$\mathcal{L} = \sum_{i}^{N} (u(x_i) - \hat{u}(x_i, \theta))^2$$



Source: [8]

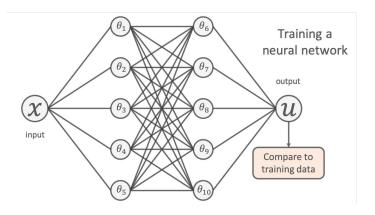




→ DNN cannot extrapolate beyond the training domain...which is exactly what we would expect from interpolation function

$$\mathcal{L} = \sum_{i}^{N} (u(x_i) - \hat{u}(x_i, \theta))^2$$

→ Go beyond data domain => more information needed:



Source: [8]



DNN cannot extrapolate beyond the training domain...which is exactly what we would expect from interpolation function

$$\mathcal{L} = \sum_{i}^{N} (u(x_i) - \hat{u}(x_i, \theta))^2$$

Go beyond data domain => more information needed:

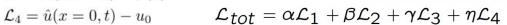
min(Loss) 🗫 Loss 🖹 Mean(data; forediction)²

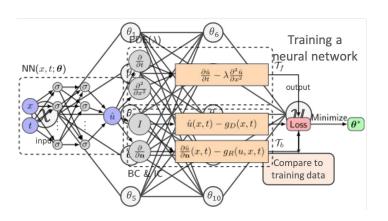
Additional_info(prediction)

$$\mathcal{L}_2 = 1/M \sum_{j=1}^{M} \left(\frac{\partial^2 \hat{u}}{\partial x^2} - \frac{\partial \hat{u}}{\partial t} \right)^2$$

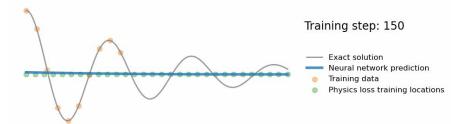
$$\mathcal{L}_3 = \hat{u}(x, t = 0) - f(x)$$

$$\mathcal{L}_4 = \hat{u}(x = 0, t) - u_0$$





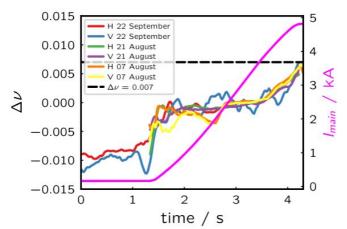


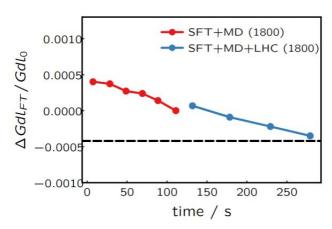


Hysteresis prediction for slow extraction



- → Hysteresis on the main SPS quadrupoles responsible for extracted beam quality degradation [9]
 - Beam based measurements highlighted tune variation
 - Magnetic measurements on spare quadrupole showed field variation compatible with beam observations

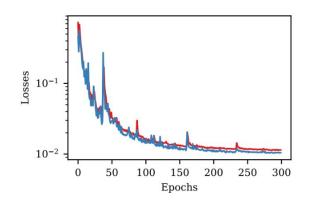


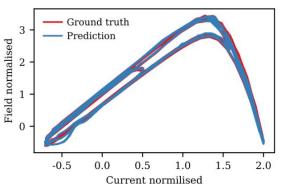


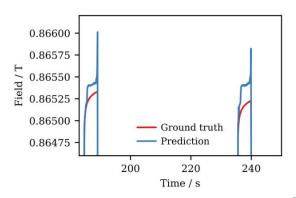
Hysteresis prediction for slow extraction



- → Hysteresis on the main SPS quadrupoles responsible for extracted beam quality degradation [9]
 - Beam based measurements highlighted tune variation
 - Magnetic measurements on spare quadrupole showed field variation compatible with beam observations
- → Classic model possible but complicated, simple NN not enough! <u>We</u> need more information!



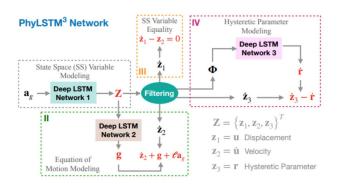




Hysteresis modelling



- → Hysteresis is rather common in physics and many other fields (chemistry, biology, economics...)
- → Modelling is rather challenging: main models Preisach and Bouc-Wen
- → In [111], PINN applied to hysteresis modelling of behaviour of structures under seismic excitation
 - This was our inspiration => very similar problem but different system
- → Here is the model used in [11]:



PINN for SPS quadrupole hysteresis



→ A generic hysteretic model can be written as [11]:

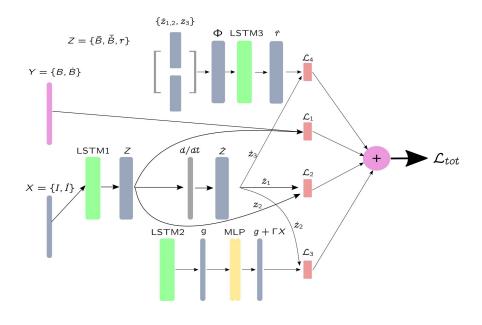
$$a\ddot{y}(t) + b(y, \dot{y}) + r(y, \dot{y}, y(\tau)) = \Gamma x(t)$$
 $\ddot{y} + g = \Gamma x$

→ Using input x = {I, dI/dt} and output y = {B, dB/dt}, we wrote our model and loss:

$$\begin{split} \mathcal{L}_1 &= \textit{MSE}(z_1(\theta_1) - y_1) + \textit{MSE}(z_2(\theta_1) - y_2) \\ \mathcal{L}_2 &= \textit{MSE}(\dot{z}_1(\theta_1) - z_2(\theta_1)) \\ \mathcal{L}_3 &= \textit{MSE}(\dot{z}_2(\theta_1) + \textit{MLP}(g(\theta_1, \theta_2), x_1)) \\ \mathcal{L}_4 &= \textit{MSE}(\dot{r}(\theta_1, \theta_3) - \dot{z}_3(\theta_1)); \dot{r} = f(\Phi); \Phi = \{\Delta z_2, r\} \end{split}$$



$$\mathcal{L}_{tot} = \alpha \mathcal{L}_1 + \beta \mathcal{L}_2 + \gamma \mathcal{L}_3 + \eta \mathcal{L}_4$$



PINN for SPS quadrupole hysteresis



- → After many attempts, we managed to train successfully one PINN for hysteresis prediction
 - Not fully optimised yet
 - Not enough data to make a proper general model for SPS quadrupoles

(fc2): Linear(in-features=350, out-features=175, bias=True) (fc21): Linear(in-features=175, out-features=1. bias=True)

(0): Linear(in-features=2, out-features=350, bias=True)

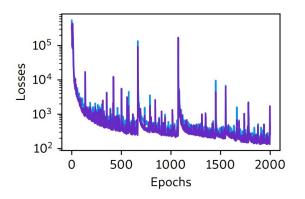
(2): Linear(in-features=350, out-features=1, bias=True))

Hyperparameters not tuned yet

PhyLSTM³

(q-plus-x): Sequential(

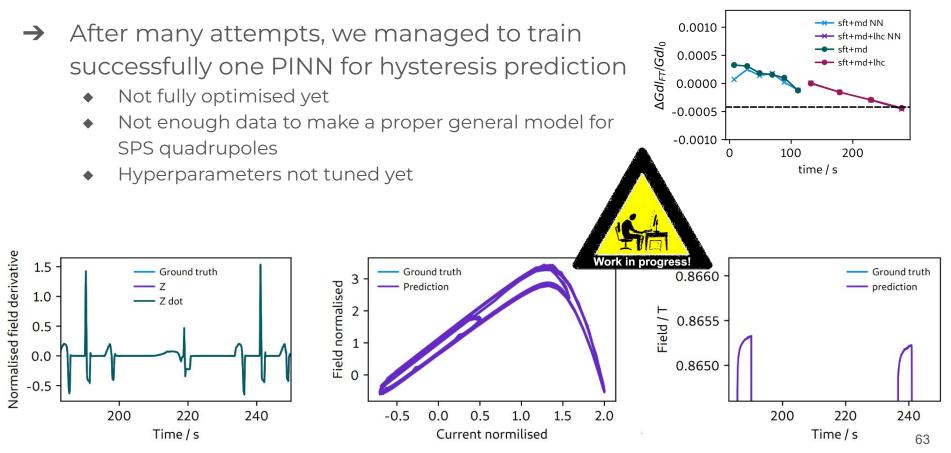
(1): ReLU()



```
(relu): LeakyReLU(negative-slope=0.01)
(lstm0): LSTM(1, 350, num-layers=3, batch-first=True, dropout=0.2)
(fc0): Linear(in-features=350, out-features=175, bias=True)
(fc01): Linear(in-features=175, out-features=3, bias=True)
(gradient): GradientTorch()
(lstm): LSTM(3, 350, num-layers=3, batch-first=True, dropout=0.2)
(fc1): Linear(in-features=350, out-features=175, bias=True)
(fc11): Linear(in-features=175, out-features=1, bias=True)
(lstm3): LSTM(2, 350, num-layers=3, batch-first=True, dropout=0.2)
```

PINN for SPS quadrupole hysteresis







- → Let's see a simple example we can quickly solve
- → Problem example:

$$u_t - Ku_{xx} = 0; 0 < x < L, t > 0$$

→ With initial and boundary conditions (Dirichlet):

$$u(x, t = 0) = f(x) \equiv x(x^2 - 3Lx + 2L^2), 0 \le x \le L$$

 $u(x = 0, t) = u(x = L, t) = 0.0, t > 0$

- → We can see in two ways:
 - Solve a IVP => PINN as PDE solver
 - u(x, t=0) = f(x) are data (it could also be x(x=0, t)) => PINN with data



- → Code example on indico: here
- → NN definition (see Andreas' slides and tutorial)
- → PDE problem definition (with derivatives)
- → Training loop



- → Code example on indico: <u>here</u>
- → <u>NN definition</u> (see Andreas' slides and tutorial)
- → PDE problem definition (with derivatives)
- → Training loop

```
class ModelNN(nn.Module):
  def __init__(self, layers=4, neurons=5):
    super(). init ()
    self.nn list = []
     for i in range(layers):
       self.nn list.append(nn.Linear(neurons, neurons))
       self.nn_list.append(nn.Sigmoid())
     self.dnn = nn.Sequential(
       nn.Linear(2, neurons),
       nn.Sigmoid(),
       *self.nn list,
       nn.Linear(neurons, 1),
  def forward(self, x, t):
    u hat = self.dnn(torch.cat([x, t], dim=-1))
     return u hat
```



- → Code example on indico: <u>here</u>
- → NN definition (see Andreas' slides and tutorial)
- → <u>PDE problem definition</u> (with derivatives)
- → Training loop

```
def diff(y, x, require graph=True):
  ones = torch.ones like(y)
  (der,) = torch.autograd.grad(
     y, x, create_graph=True, grad_outputs=ones, allow_unused=True
  if require_graph:
     der.requires grad ()
  return der
K = 0.3
L = 2
def pde(x, t, model):
  u hat = model(x, t)
  u x = diff(u hat, x)
  u xx = diff(u x, x)
  u t = diff(u hat, t)
  return u t-K*u xx
def u_ic_f(x):
  return x * (x**2 - 3 * L * x + 2 * L**2)
```



- → Code example on indico: <u>here</u>
- → NN definition (see Andreas' slides and tutorial)
- → PDE problem definition (with derivatives)
- → <u>Training loop</u>

```
pde_target = torch.zeros((500, 1)).to(dev)

x_ic = torch.rand((500, 1)).to(dev) * L

t_ic = torch.zeros((500, 1)).to(dev)

u_ic = u_ic_f(x_ic)

x_bc = torch.zeros((500, 1)).to(dev) + L

x_bc_2 = torch.zeros((500, 1)).to(dev)

t_bc = torch.rand((500, 1)).to(dev)

u_bc = 0.0 * t_bc

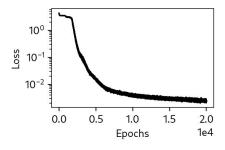
u_bc_2 = 0.0 * t_bc

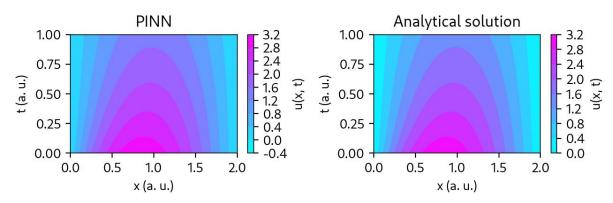
epochs = 20000
```

```
losses = []
progress bar = trange(epochs, unit="epoch")
for epoch in progress bar:
  optimiser.zero_grad()
  u bc hat = model nn(x bc, t bc)
  I_bc = mse_loss(u_bc_hat, u_bc)
  u_bc_2hat = model_nn(x_bc_2, t_bc)
  I bc 2 = mse loss(u bc 2 hat, u bc 2)
  u ic hat = model nn(x ic, t ic)
  I ic = mse loss(u ic hat, u ic)
  t = torch.rand((500, 1)).to(dev)
  t.requires grad = True
  x = torch.rand((500, 1)).to(dev) * L
  x.requires_grad = True
  pde hat = pde(x, t, model nn)
  I pde = mse loss(pde hat, pde target)
  loss = lic + lpde + lbc + lbc 2
  loss.backward()
  optimiser.step()
  losses.append(loss.item())
  progress bar.set postfix(loss=loss.item())
                                        68
```



- → Results as compared with analytical solution
 - ♦ Indistinguishable!
- → Caveats:
 - Training takes quite some time (well, not in this particular case!)
 - With data, need to balance properly the different loss function components
- → Easily possible to extend to inhomogeneous cases





Summary



- → CNNs can be used quite effectively in the accelerator complex
 - First results very promising
- → LSTM-based models used for kicker heating predictions and hysteresis modelling
 - Physics loss fundamental for low data
- → PINN introducing a new way to train NN
 - Include more information via problem definition and a priori knowledge
 - Great for "extrapolation"
 - ◆ Still quite a lot to explore, for example Maxwell equations solved with NN [12]
- → What's coming next?
 - ◆ Transformer (or attention) based NN are destroying the competition in <u>NLP</u>, <u>time</u> <u>series forecasting</u>, <u>image classification</u>... => we should look into this ASAP!



Thank you very much!