

9<sup>th</sup> November 2022

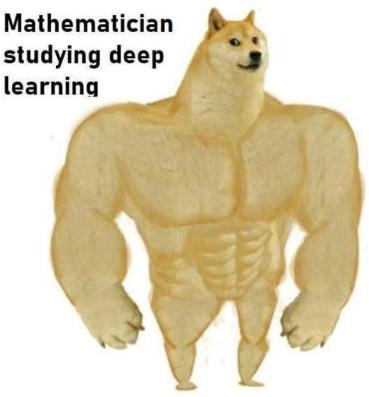
## ML 4 Time-series: Recurrent Neural Networks

Dr. Andrew P. Creagh | Dr. Anshul Thacker | Prof. David A. Clifton

Institute of Biomedical Engineering (IBME),
Department of Engineering Science,
Old Road Campus Research Building (ORCRB),
University of Oxford



### CDT in Health Data Science



Boy, am I glad I studied linear algebra, numerical optimisation, measure theory, and convex optimisation during my undergrad. This sure would be difficult without it

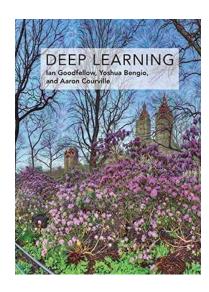
Deep learner studying the maths



Wot's chaim rool?

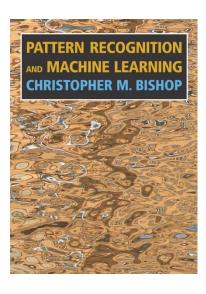
Credit: https://www.facebook.com/convolutionalmemes/

### Resources



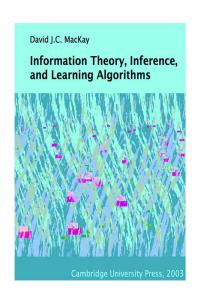
A well-written introduction to all things deep learning (DL), from leaders in the field of theoretical DL.

Very light maths



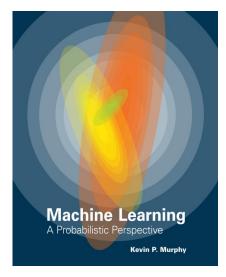
A core classic describing most non-DL algorithms. Very good for one's general understanding.

Reasonably "maths-y"



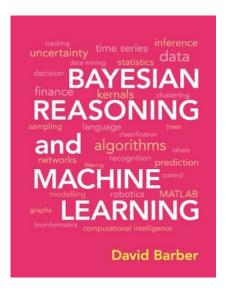
Another core classic, from one of the field's (sadly departed) foundational thinkers – good, even though it's from Cambridge

Reasonably "maths-y"



Seriously comprehensive, one of the best books for general machine learning. Excellent examples.

Really rather "maths-y"



Big, bad, and Bayesian. Everything you'd like to know about Bayesian machine learning. Great for time-series analysis.

Seriously "maths-y"

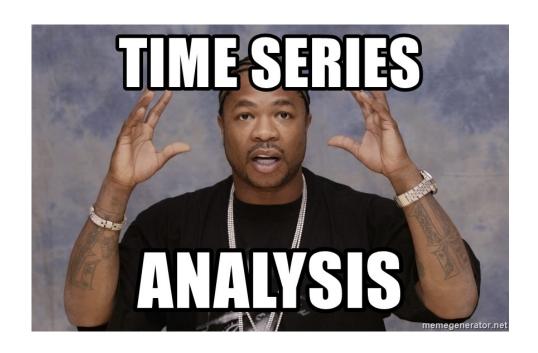


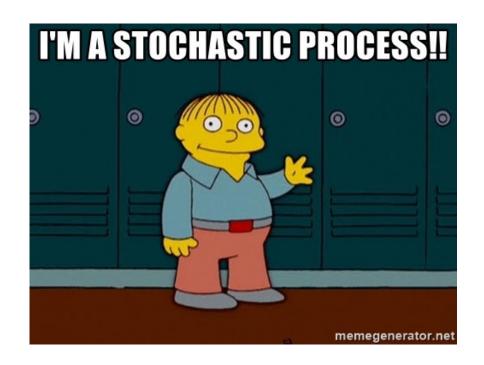
mild medium hot extra hot

# Why time?



Clinical data is **not** static: clinical measurements are often a time-series, (e.g. heart rate) or repeated measurements taken during visits to the doctor, or a stay in hospital. Clinical events can occur at a point in time (e.g. a heart attack) or can even be causal. These events generally evolve over time (known as **Stochastic processes**)





# Choosing your model

#### Models that don't consider time (i.i.d.)

- Linear / Logistic Regression
- Support Vector Machines (SVM)
- Classification and Regression Trees (CART) (e.g. Random Forest)
- eXtreme Gradient Boosting (XGBoost)
- Deep Neural Networks
- Etc.

Need to incorporate time through the features instead!

#### Choose your fighter!



Image Credit

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#### Models that consider time (non i.i.d)

- Markov Chains
- Autoregressive Processes
- Hidden Markov Models (HMM)
- Recurrent Neural Networks (RNN) / Long-Short Term Memory (LSTM)
- Transformers,
- Etc.

#### Choose your fighter!



**Image Credit** 

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#### Choose your fighter!



Image Credit

#### Is a more complex model *necessary*?



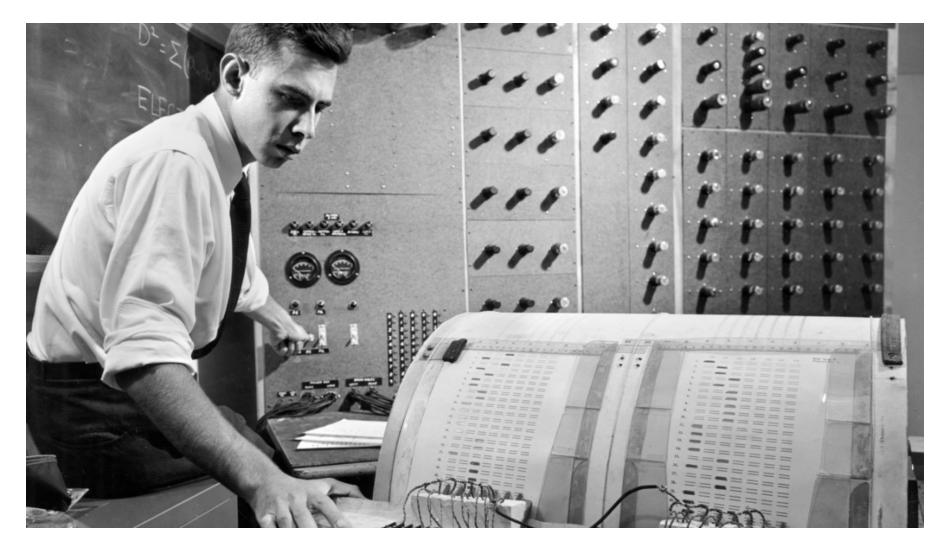


The importance of data curation, cleaning, and preprocessing are often overlooked



#### Sequential learning using memorisation

- From perceptron to multi-layer perceptron
- Neurons with recurrence
- RNNs
- The problems with long-term dependencies
- Gating to memorize long-term dependencies
- LSTMs
- Sequence processing



Frank Rosenblatt 1950, Ph.D. 1956, works on the "perceptron" – what he described as the first machine "capable of having an original idea."

## The Perceptron



REPORT NO. 85-460-1

THE PERCEPTRON

A PERCEIVING AND RECOGNIZING AUTOMATON

(PROJECT PARA)

January, 1957

Prepared by: Frank Roserblatt

Frank Rosenblatt, Project Engineer

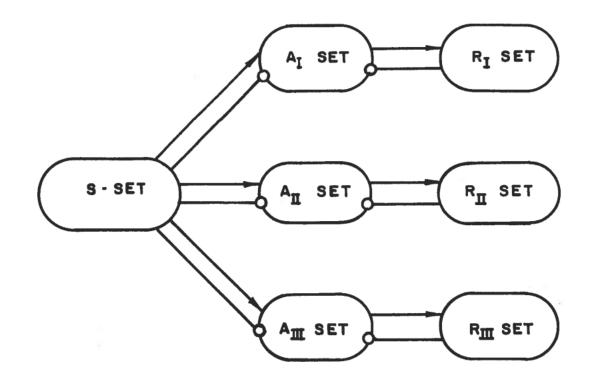
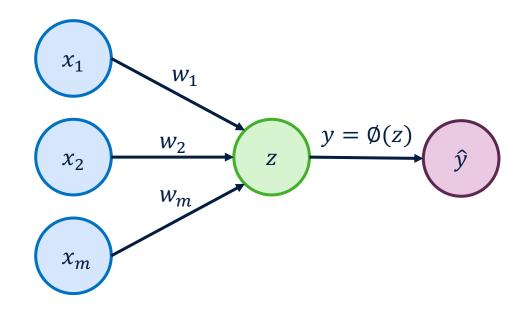


FIGURE 2
ORGANIZATION OF A PERCEPTRON WITH
THREE INDEPENDENT OUTPUT-SETS

## The Perceptron

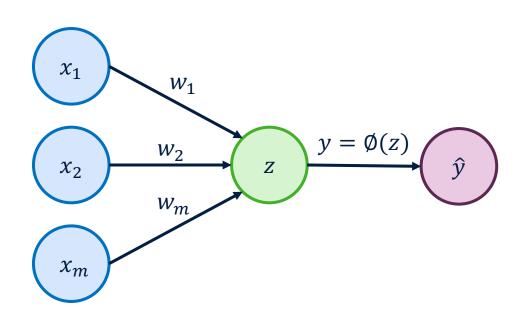
The perceptron is the building block to modern day feed-forward deep networks. A perceptron layer takes a weighted linear combination (sum) of the inputs  $\mathbf{x} \in \mathbb{R}^m$  and transform this to an output through some (often non-linear) positive and monotonically increasing activation function  $\emptyset(\cdot)$  to yield a prediction or output  $\hat{y}$ 



$$\mathbf{x} \in \mathbb{R}^m$$
  $z = \mathbf{w}^\mathsf{T} \mathbf{x}$   $\widehat{\mathbf{y}} = \emptyset(\mathbf{w}^\mathsf{T} \mathbf{x})$ 

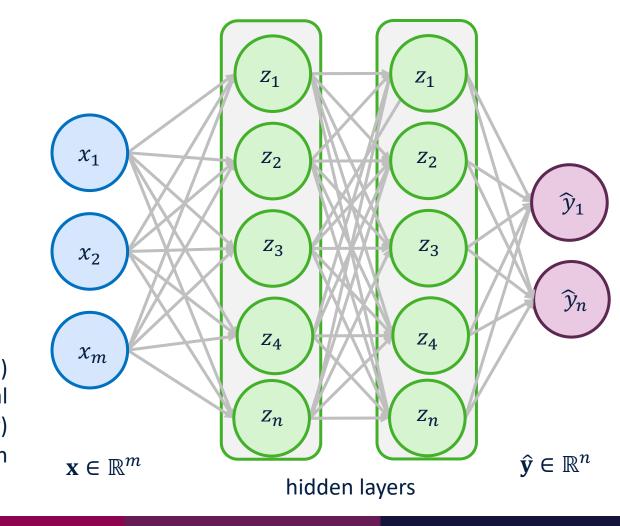
## Advancing towards deep networks

the perceptron

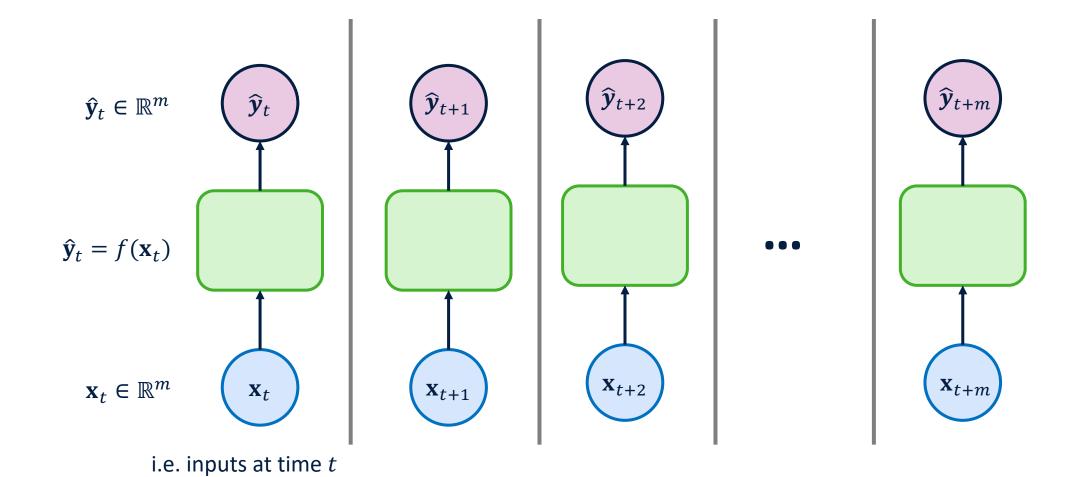


Deep learning typically describes multi-layer perceptron (MLP) blocks that are stacked in cascading architectural arrangements, consisting of a number of (often non-linear) functions successively layered together, which map an input  ${\bf x}$  to some output  ${\bf y}$ 

MLP, feed forward networks



## Treating individual time-steps as I.I.D.

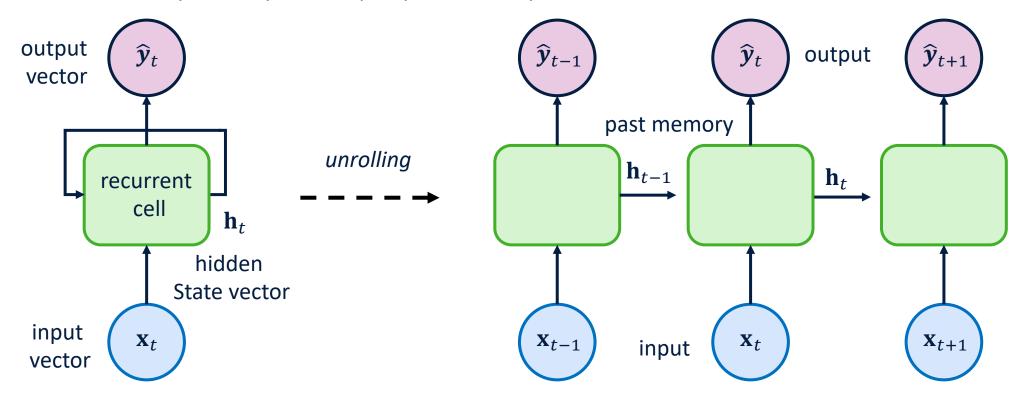


time

I.I.D: Independent and identically distributed

### Neurons with Recurrence

Apply a recurrence cell step at every time step to process a sequence



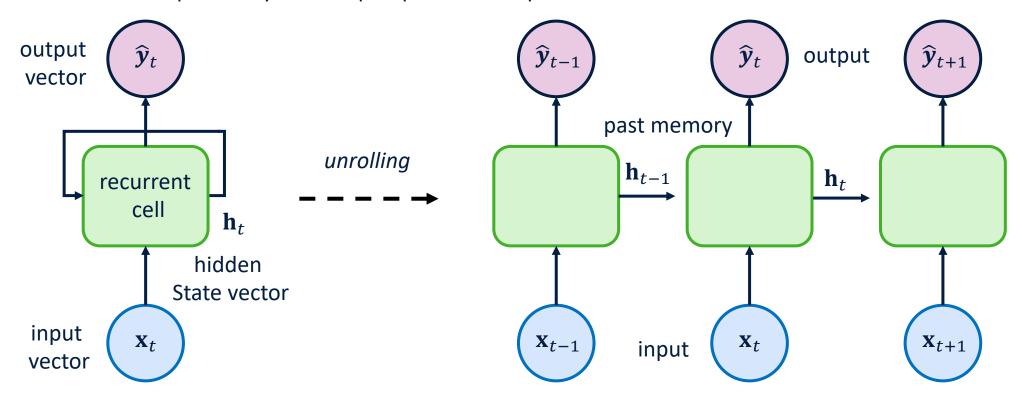
RNNs have a state  $\mathbf{h}_t$ , that is updated at each time step as a sequence is processed

1) **rolled** network



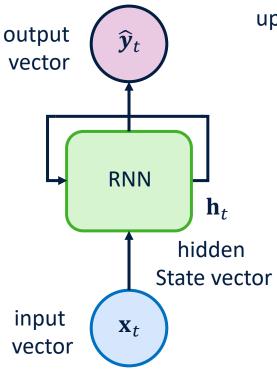
### Neurons with Recurrence

Apply a recurrence cell step at every time step to process a sequence

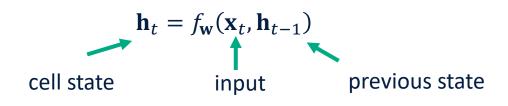




Apply a recurrence cell step at every time step to process a sequence



update the hidden state using function with weights w



$$\mathbf{h}_t = \tanh \left( \mathbf{W}_{\mathbf{h}\mathbf{h}}^T \mathbf{h}_{t-1} + \mathbf{W}_{\mathbf{x}\mathbf{h}}^T \mathbf{h}_t \right)$$

$$\hat{\mathbf{y}}_t = \mathbf{W}_{\mathbf{h}\mathbf{y}}^T \mathbf{h}_t$$
 (output vector)

**W**<sub>hh</sub>: recurrent weights

**W**<sub>hy</sub>: hidden weights

 $W_{xh}$ : input weights

Apply a recurrence cell step at every time step to process a sequence

 $\mathbf{h}_t$ 

hidden

State vector

cell state

output

vector

input

vector

**RNN** 

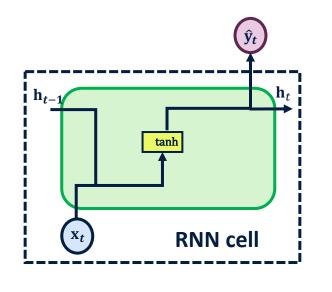
 $\mathbf{X}_t$ 

update the hidden state using function with weights  ${f w}$ 

 $W_{hh}$ : recurrent weights

**W**<sub>hy</sub>: hidden weights

 $W_{xh}$ : input weights



$$\mathbf{h}_t = f_{\mathbf{w}}(\mathbf{x}_t, \mathbf{h}_{t-1})$$

$$\mathbf{h}_t = \tanh(\mathbf{W}_{\mathbf{h}\mathbf{h}}^T \mathbf{h}_{t-1} + \mathbf{W}_{\mathbf{x}\mathbf{h}}^T \mathbf{h}_t)$$

$$\hat{\mathbf{y}}_t = \mathbf{W}_{\mathbf{h}\mathbf{y}}^T \mathbf{h}_t \quad \text{(output vector)}$$

Apply a recurrence cell step at every time step to process a sequence

update the hidden state using function with weights **w** 

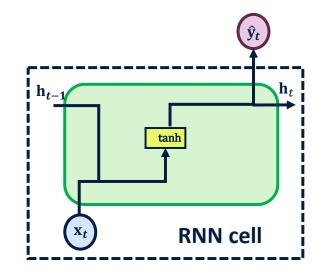
 $W_{hh}$ : recurrent weights

 $W_{hy}$ : hidden weights

 $W_{xh}$ : input weights

minimal code example

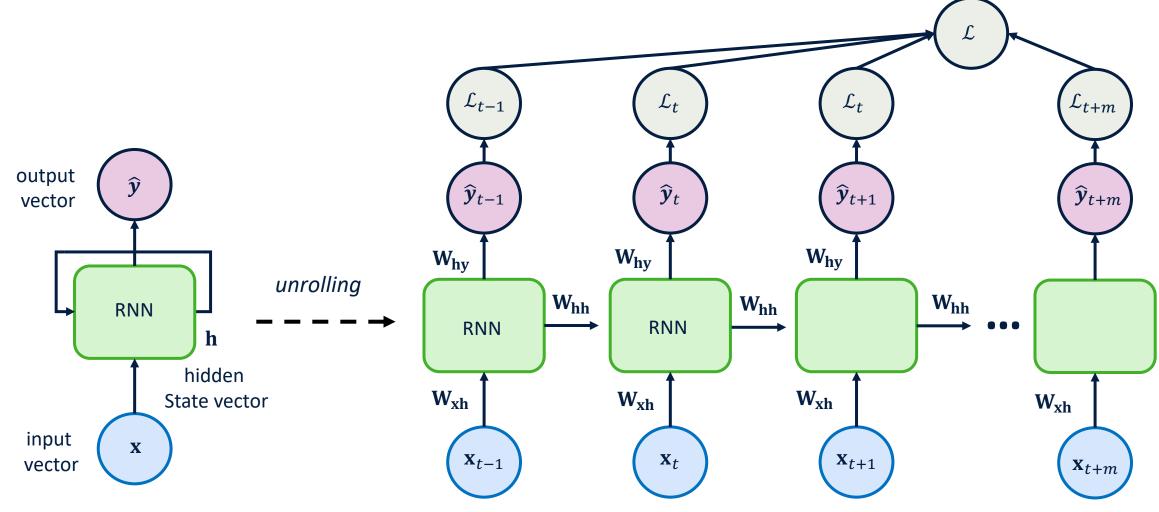
```
class RNN:
    # ...
    def step(self, x):
        # update the hidden state
        self.h =
        np.tanh(np.dot(self.W_hh, self.h)
        + np.dot(self.W_xh, x))
        # compute the output vector
        y = np.dot(self.W_hy, self.h)
        return y
```



$$\mathbf{h}_t = \tanh(\mathbf{W}_{\mathbf{h}\mathbf{h}}^T \mathbf{h}_{t-1} + \mathbf{W}_{\mathbf{x}\mathbf{h}}^T \mathbf{h}_t)$$

 $\mathbf{h}_t = f_{\mathbf{w}}(\mathbf{x}_t, \mathbf{h}_{t-1})$ 

$$\hat{\mathbf{y}}_t = \mathbf{W}_{\mathbf{h}\mathbf{y}}^T \mathbf{h}_t$$
 (output vector)

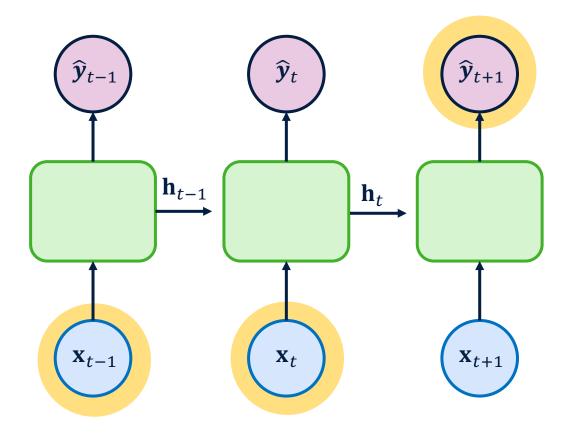


represent as a computational graph unrolled across time

**W**<sub>hv</sub>: hidden weights

**W**<sub>hh</sub>: recurrent weights

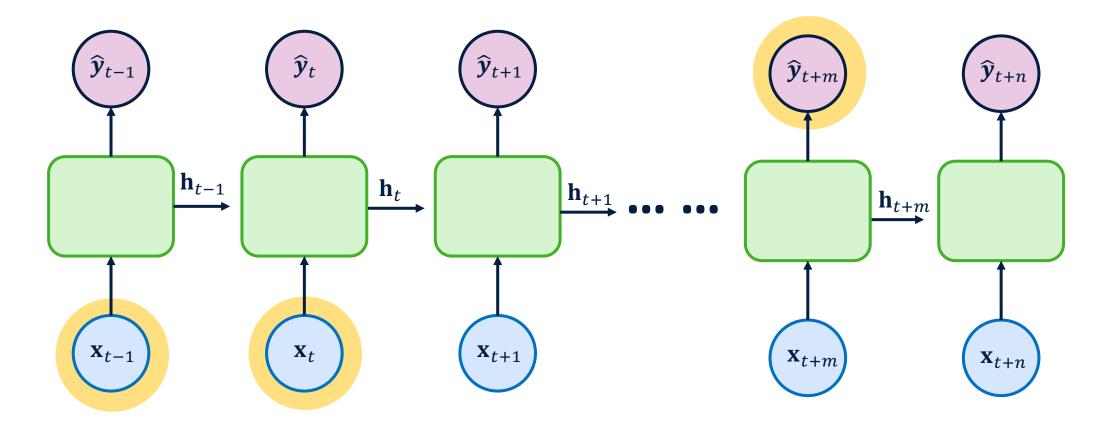
# The Problem of Long-Term Dependencies



In cases certain cases, such as where the gap between the relevant information and the place that it's needed is small, RNNs can learn to use the past information.

"The clouds are in the \_\_\_\_"

# The Problem of Long-Term Dependencies



"I grew up in France, .....,

and I speak fluent \_\_\_\_ "

# The Problem of Long-Term Dependencies

Problems of long-term information flow...

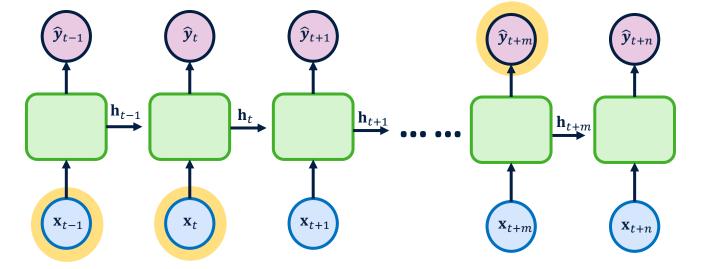
**Exploding and Vanishing Gradients**: Computing the gradient  $\nabla$ (to train the model) w.r.t.  $\mathbf{h}_t$  often requires many factors of  $\mathbf{W_{hh}}$  and repeated gradient computation!

many values of:

$$\nabla_{\mathbf{h}_t} \gg 1$$

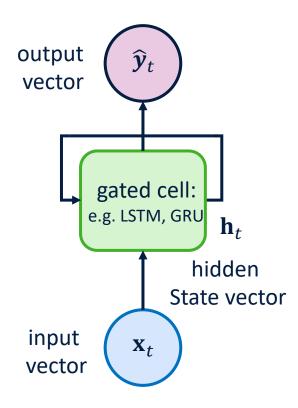
$$\nabla_{\mathbf{h}_t} \ll 1$$

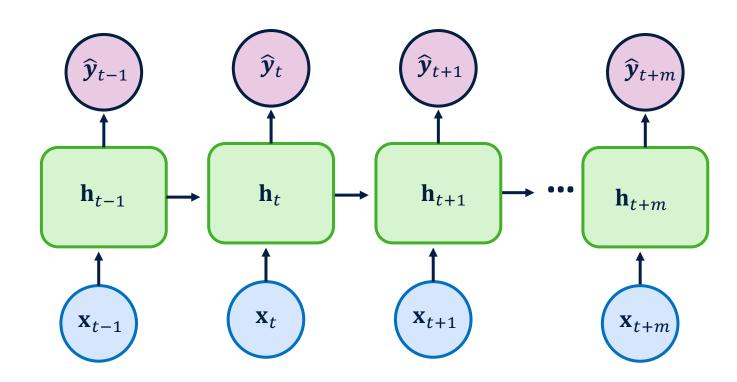
exploding gradients vanishing gradients



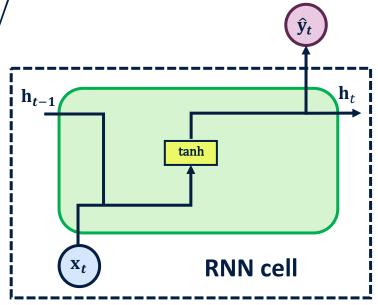
...multiply many small numbers together  $\rightarrow$  errors due to further back time steps have smaller and smaller gradients  $\rightarrow$  bias parameters to capture short-term dependencies

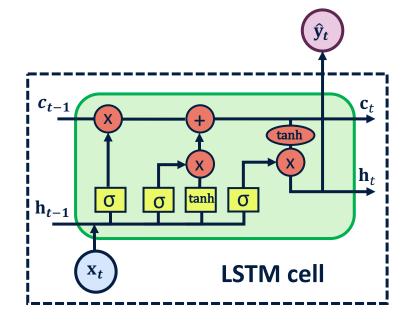
# Gating to memorize long-term dependencies

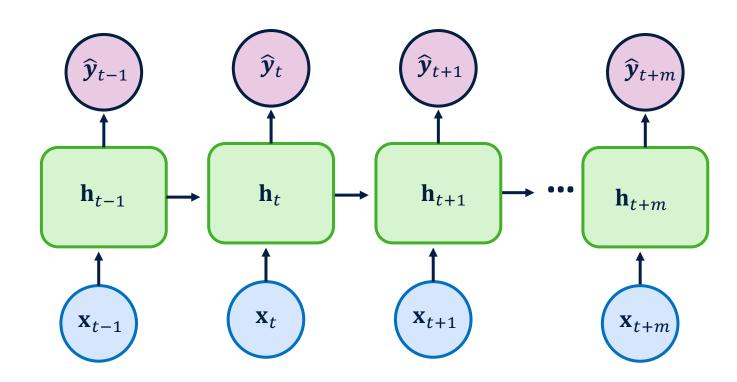




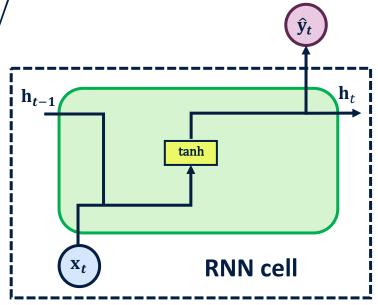
- RNN contains simple computation node
- Replace with LSTM computation block with control information flow (memory)
- LSTMS can track information over many (t + m) timesteps

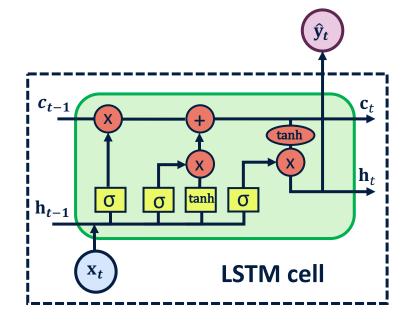


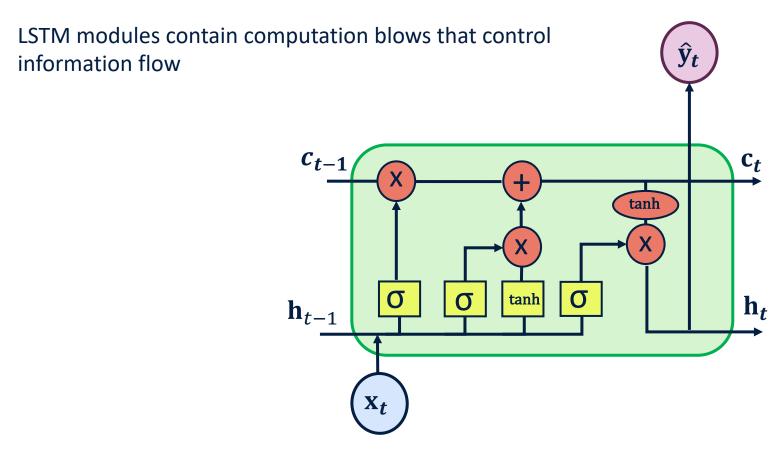




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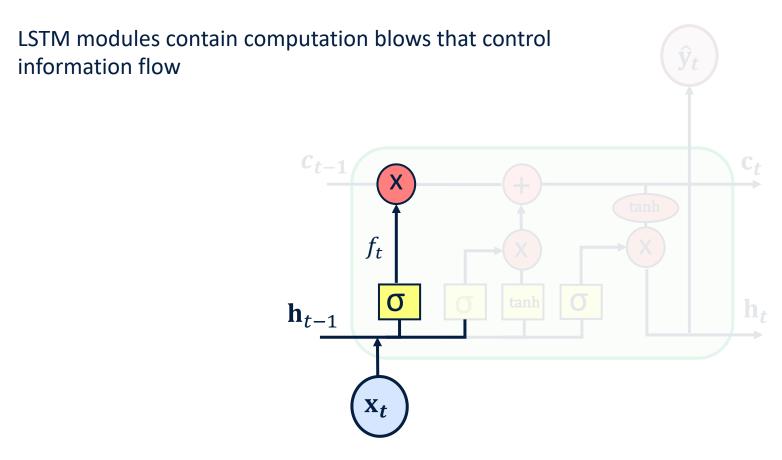






- X : pointwise multiplication
- +: pointwise addition
- σ: sigmoid function
- tanh: hyperbolic tangent function

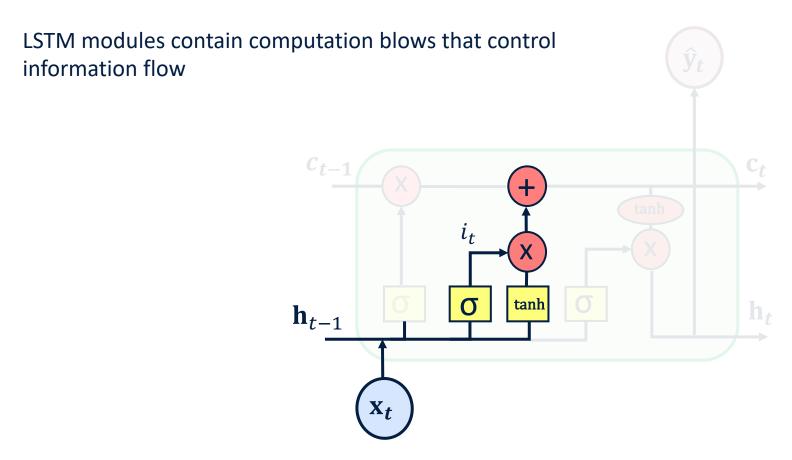
1) Forget 2) Store 3) Update 4) Output



- X : pointwise multiplication
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1) Forget 2) Store 3) Update 4) Output

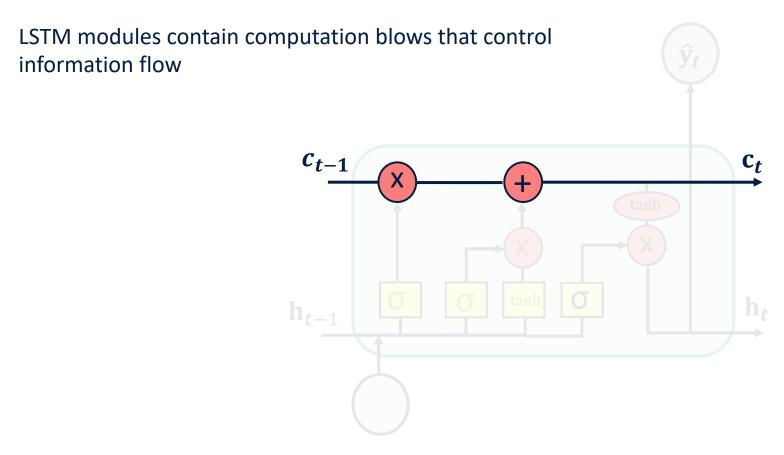
LSTMs forget irrelevant parts of the previous state



- X : pointwise multiplication
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1) Forget 2) Store 3) Update 4) Output

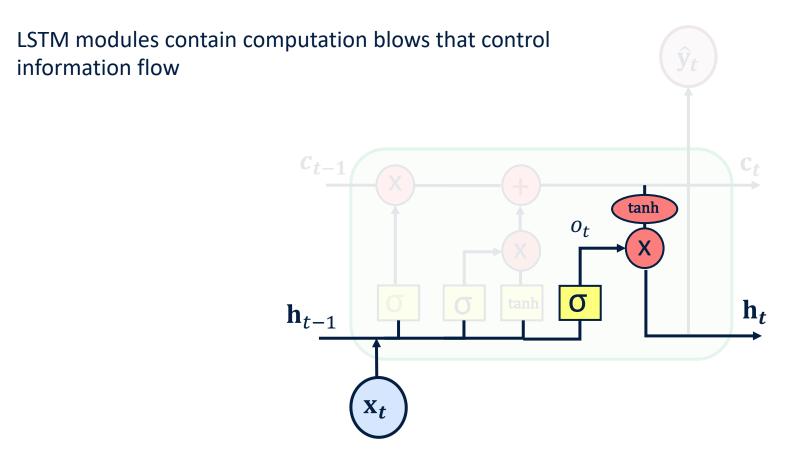
LSTMs store relevant new information into the cell state



- X : pointwise multiplication
- +: pointwise addition
- σ: sigmoid function
- tanh: hyperbolic tangent function

1) Forget 2) Store 3) Update 4) Output

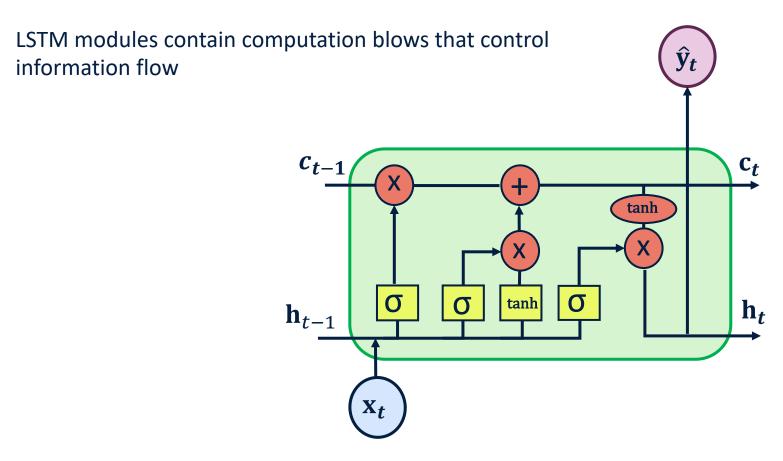
LSTMs **selectively update** cell state values



- X : pointwise multiplication
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1) Forget 2) Store 3) Update 4) Output

LSTMs output gate controls what information is sent to the next step, essentially returning a filtered version of the cell state



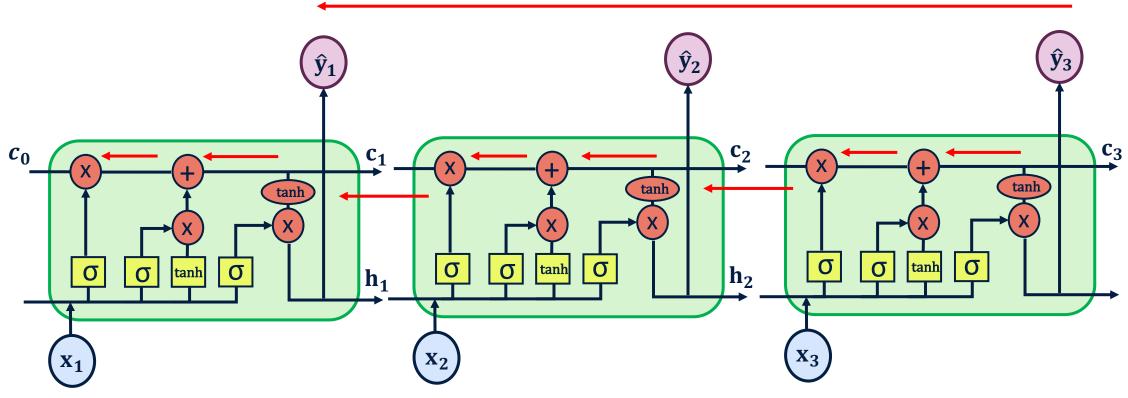
- X : pointwise multiplication
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- σ: sigmoid function
- tanh: hyperbolic tangent function

1) Forget 2) Store 3) Update 4) Output

Key Concept: LSTMS maintain a separate cell state from what is outputted and uses gates to control the flow of information

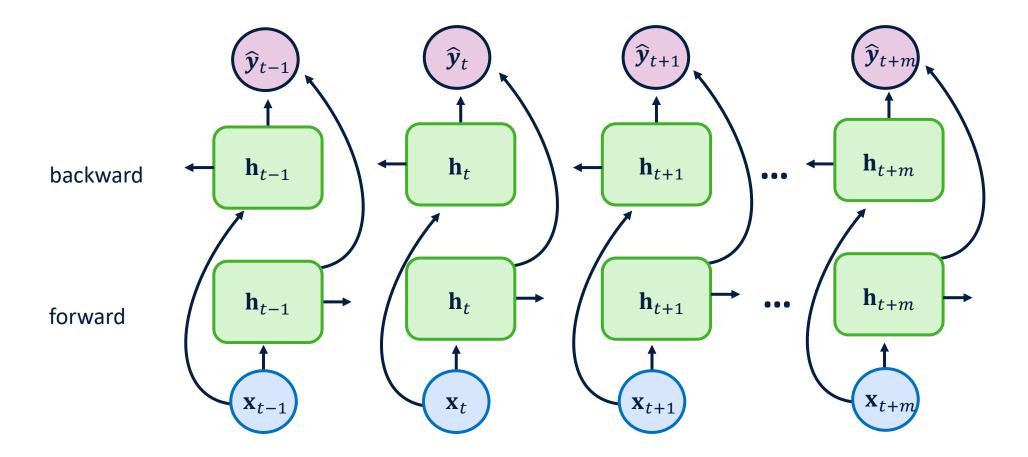
Forward pass  $\mathbf{c}_{\mathbf{2}}$  $\mathbf{c}_3$ tanh tanh tanh tanh tanh  $h_2$  $h_1$ 

Uninterrupted gradient flow overcomes vanishing gradient problem



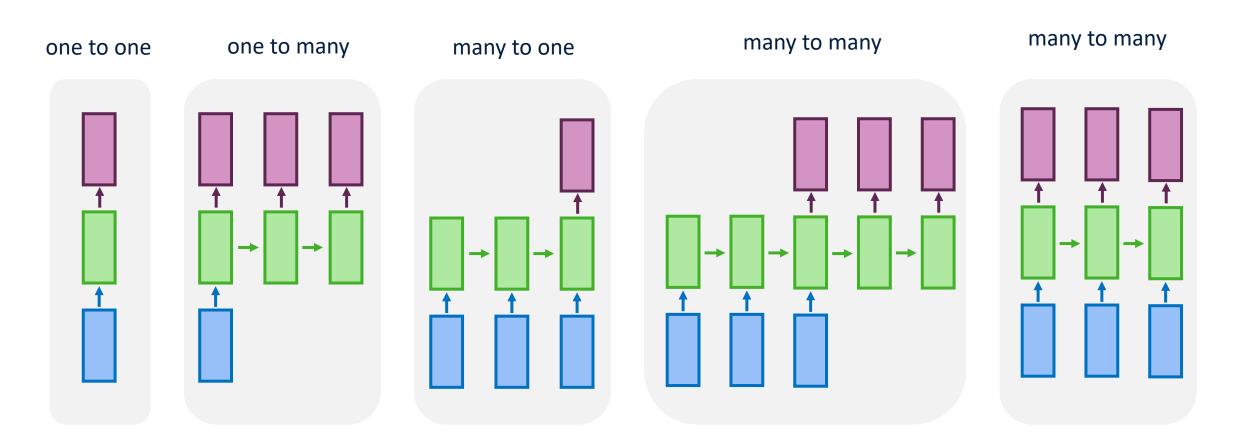
**Key Concept:** No multiplication with weights matrix  $\mathbf{W}$  during backpropagation (don't worry about this too much!) Cell state multiplied by different values of forget gate  $\rightarrow$  less prone to vanishing and exploding gradient problems

### Bi-directional RNNs



The hidden state is the concatenated result of both forward and backward hidden states so that it can capture past and future information

# Sequence Processing Options



Source: <a href="https://karpathy.github.io/2015/05/21/rnn-effectiveness/">https://karpathy.github.io/2015/05/21/rnn-effectiveness/</a>

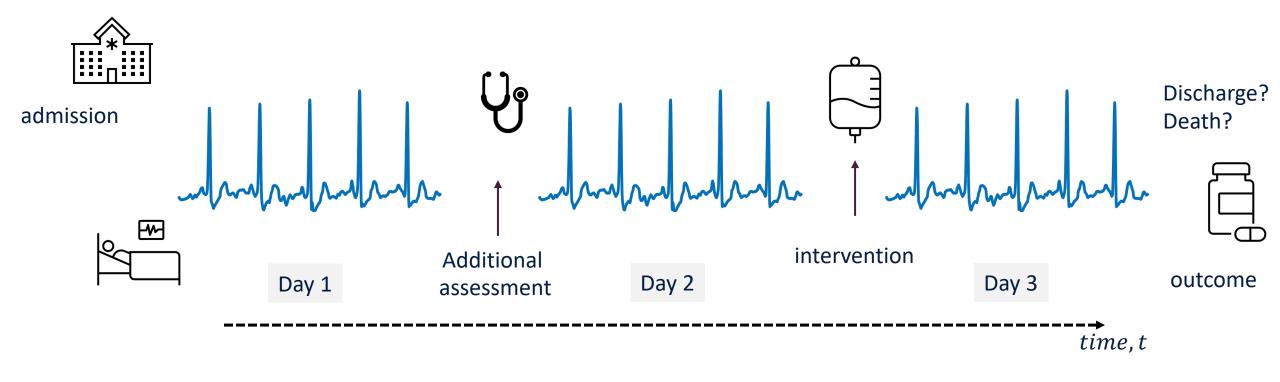


## How to implement RNNs?

#### The practicalities:

- 1. Understanding your problem
- 2. Setting up your RNN
- 3. Picking your ML framework
- 4. Training your RNN
- 5. Avoiding overfitting
- 6. Your machine learning pipeline

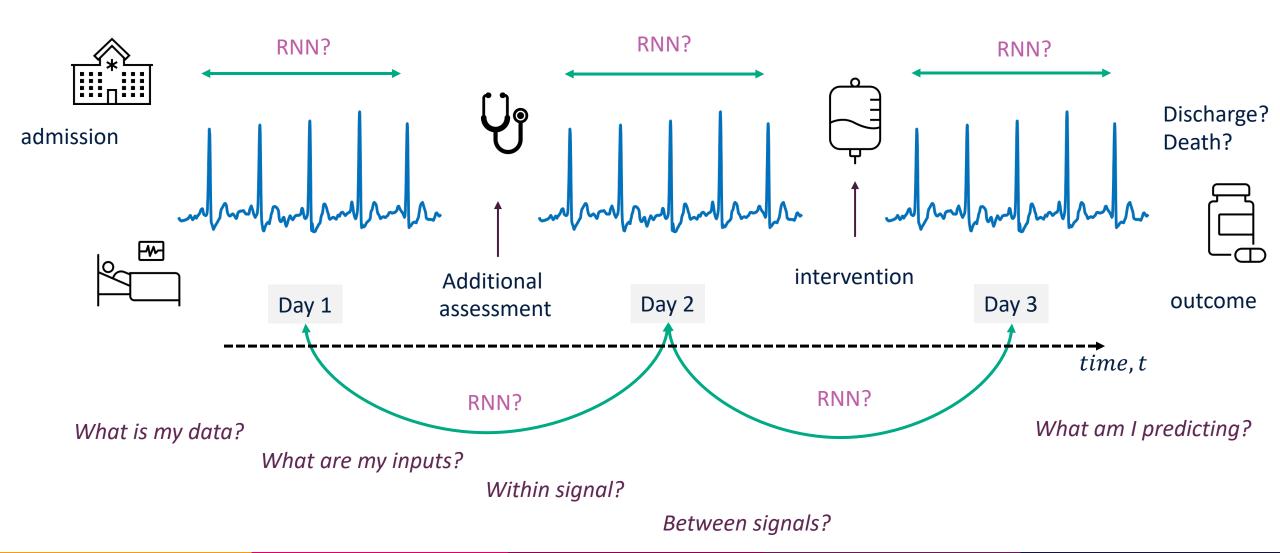
## Setting up your time-series problem

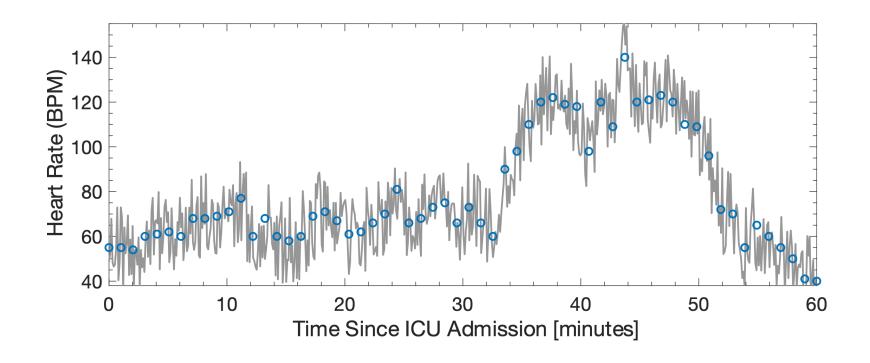


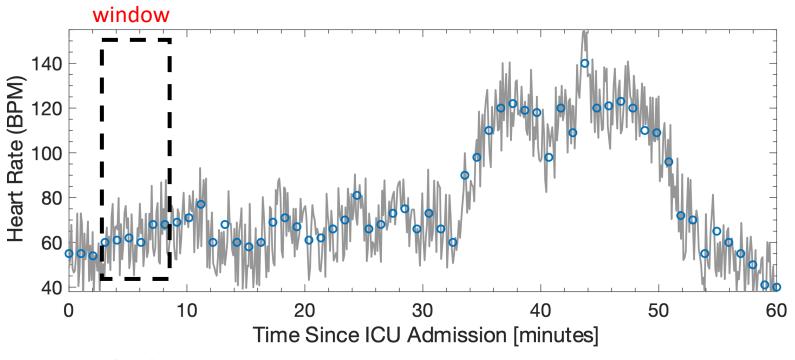
What is my data?

What am I predicting?

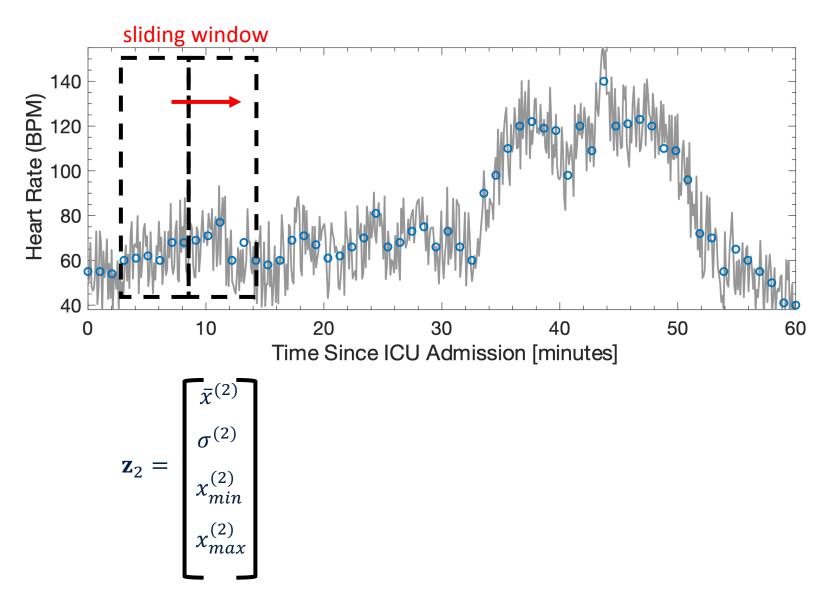
## Setting up your time-series problem

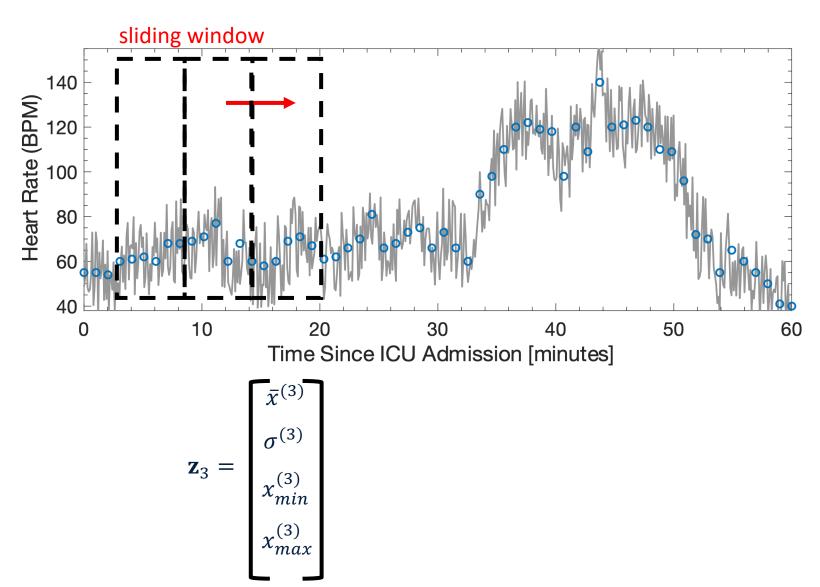


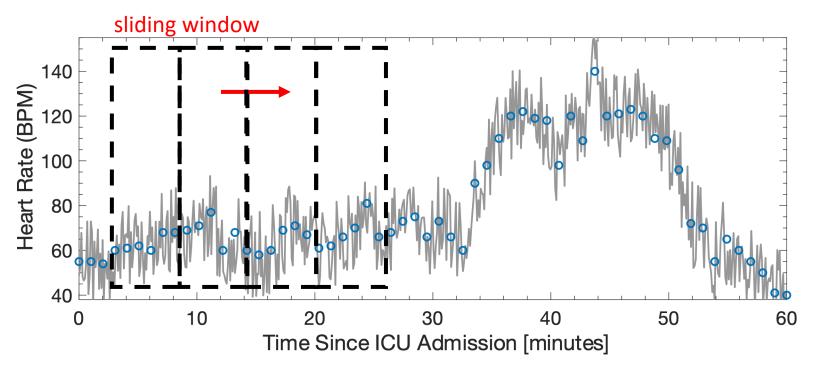




$$\mathbf{z}_{1} = \begin{bmatrix} \bar{x}^{(1)} \\ \sigma^{(1)} \\ x_{min}^{(1)} \\ x_{max}^{(1)} \end{bmatrix}$$

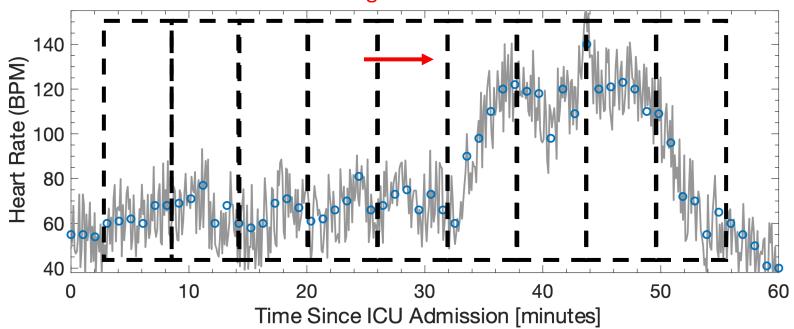






$$\mathbf{z}_{3} = \begin{bmatrix} \bar{x}^{(3)} \\ \sigma^{(3)} \\ x_{min}^{(3)} \\ x_{max}^{(3)} \end{bmatrix}$$

#### sliding window



$$\mathbf{z}_{m} = \begin{bmatrix} \bar{x}^{(m)} \\ \sigma^{(m)} \\ x_{min}^{(m)} \\ x_{max}^{(m)} \end{bmatrix}$$

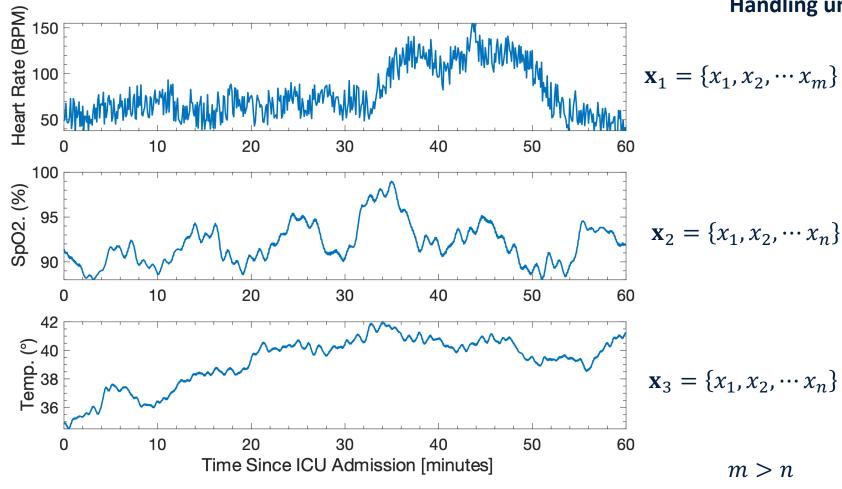
$$\mathbf{z}_{m} = \left[\bar{x}^{(m)}, \sigma^{(m)}, x_{min}^{(m)}, x_{max}^{(m)}\right]^{\mathrm{T}}$$

$$\mathbf{Z} = [\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3, \cdots, \mathbf{z}_T]$$

$$\mathbf{Z} \in \mathbb{R}^{P \times T}$$

*P*: number of features, input channels, etc. *T*: number of timesteps.

### Handling Multivariate Time-Series Data

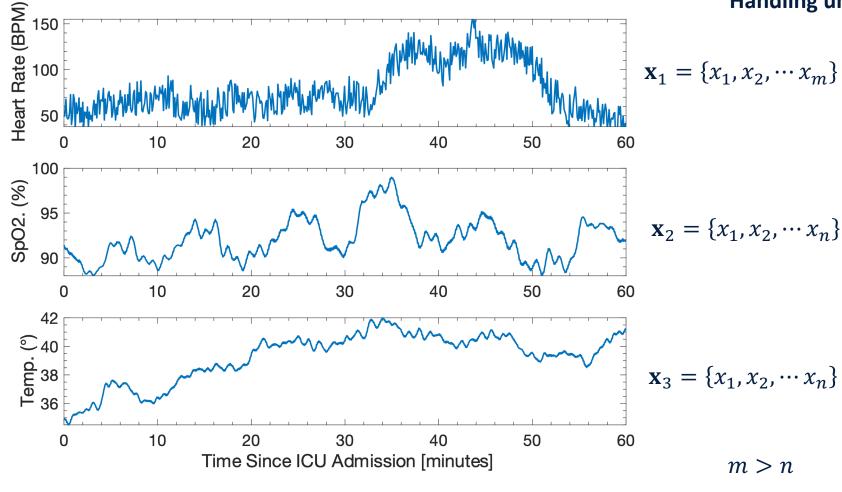


#### Handling uneven / irregularly sampled data:

#### Resampling

- Downsample (or window)
- Don't up-sample (if you can avoid it); you're interpolating information that you don't know, which is always dangerous

### Handling Multivariate Time-Series Data



#### Handling uneven / irregularly sampled data:

#### Resampling

- Downsample (or window)
- Don't up-sample (if you can avoid it); you're interpolating information that you don't know, which is always dangerous

$$\mathbf{Z} \in \mathbb{R}^{P \times T}$$

for each time-series feature (e.g. HR, SpO2, Temp.)

$$\mathbf{Z} \in \mathbb{R}^{(P \times 3) \times T}$$

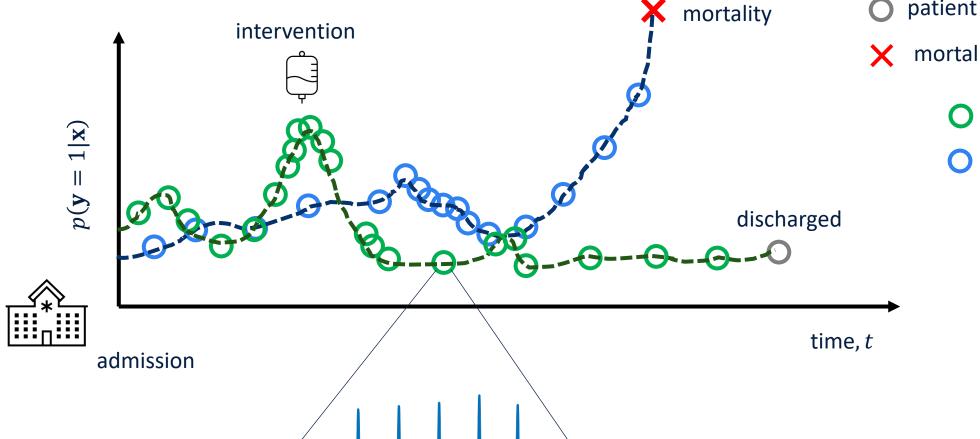
### ICU admission problem

After 3 days, is the patient alive or dead, m = 5 days?



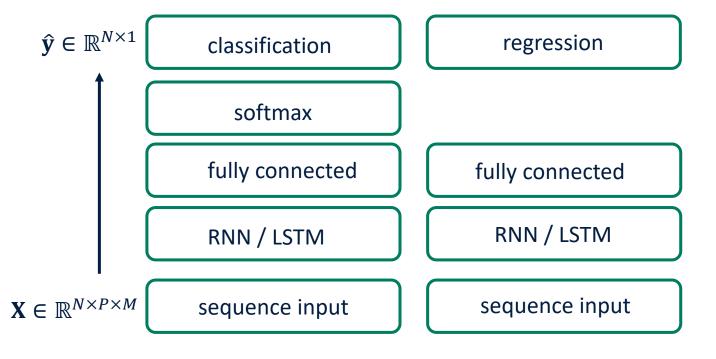
$$\times$$
 mortality  $(y = 1)$ 

- Patient #1
- Patient #2



5 mins

# Setting up your RNN



*N*: number of samples / observations.

*M*: number of timesteps.

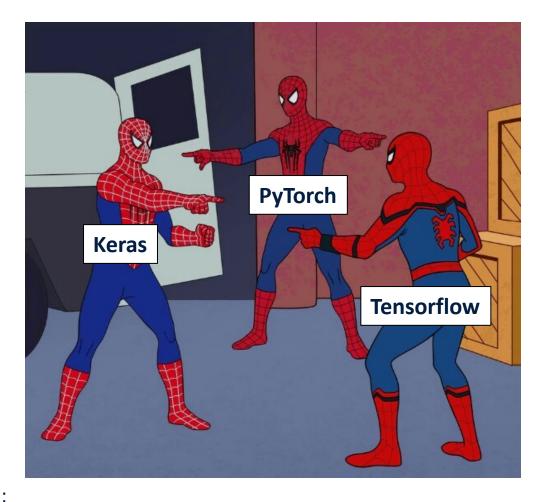
P: number of features, input channels, etc.

#### Input data considerations:

LSTM networks support input data with varying sequence lengths.

- Padding: add values (usually zeros) to the start/end of sequences so that all the sequences have the same length as the longest/shortest sequence
- Truncating: make all sequences the same length as the shortest sequence. The remaining data in the sequences is discarded.
- Splitting: pads all the sequences to the nearest multiple of the specified length that is greater than the longest sequence length. Then, split each sequence into smaller sequences of the specified length

### What framework to use?\*



For some good comparison information:

https://www.projectpro.io/article/pytorch-vs-tensorflow-2021-a-head-to-head-comparison/416 https://medium.com/analytics-vidhya/ml03-9de2f0dbd62d

### LSTM example

N = 500: number of samples / observations.

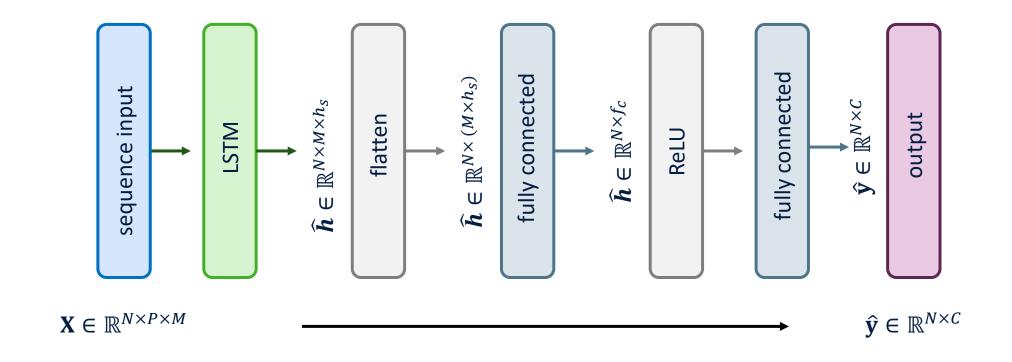
M = 10: number of timesteps

P = 3: number of features, input channels, etc.

C = 6: number of classes

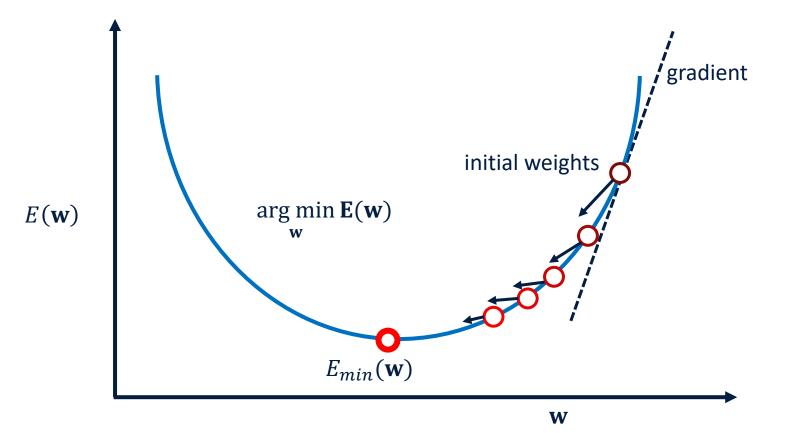
 $h_S = 128$ : hidden size

 $f_c = 64$ : number of fully connected nodes



### LSTM example code

```
import torch #pytorch
import torch.nn as nn
from torch.autograd import Variable
class Model(nn.Module);
     def __init__(self, num_classes=3, input_size=3, hidden_size=128, num_layers=1, seq_length=10):
          super(model, self). init ()
          self.num classes = num classes #number of classes
          self.num_layers = num_layers #number of recurrent layers
          self.input_size = input_size #input size (# features / channels)
          self.hidden_size = hidden_size #hidden state
          self.seg length = seg length #sequence length
          self.lstm = nn.LSTM(input_size=input_size, hidden_size=hidden_size,
                    num_layers=num_layers, batch_first=True) #lstm
          self.fc_1 = nn.Linear(hidden_size, 100) #fully connected 1
          self.fc = nn.Linear(100, num classes) #fully connected last layer
          self.relu = nn.ReLU()
     def forward(self,x):
          h_0 = Variable(torch.zeros(self.num_layers, x.size(0), self.hidden_size)) #hidden state
          c_0 = Variable(torch.zeros(self.num_layers, x.size(0), self.hidden_size)) #internal state
          # Propagate input through LSTM
          output, (hn, cn) = self.lstm(x, (h_0, c_0)) #lstm with input, hidden, and internal state
          hn = hn.view(-1, self.hidden_size) #reshaping the data for Dense layer next
          out = self.fc 1(hn) #first Dense
          out = self.relu(out) #relu
          out = self.fc(out) #Final Output
          return out
```



**Jacobian** 

gradient 
$$\mathbf{J} = \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = \nabla E(\mathbf{w})$$

Hessian

$$\mathbf{H} = \frac{\partial^2 E(\mathbf{w})}{\partial \mathbf{w} \partial \mathbf{w}^{\mathsf{T}}} = \nabla^2 E(\mathbf{w})$$

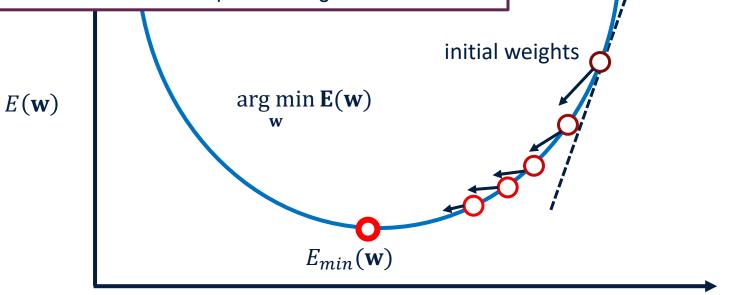
We can use Newton-Raphson

$$x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$$

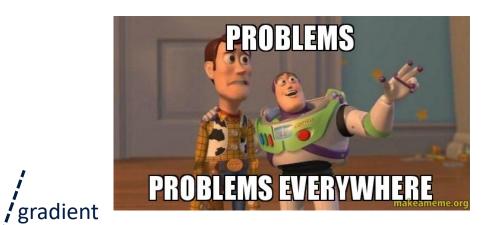
#### Training a model, TL;DR:

#### **But I'm not using Logistic Regression?**

Newton-Raphson is computationally expensive as it requires solving the second derivative Hessian **H**, which can be intractable and attracts saddle points in higher dimensions...



W



#### **Jacobian**

$$\mathbf{J} = \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = \nabla E(\mathbf{w})$$

#### Hessian

$$\mathbf{H} = \frac{\partial^2 E(\mathbf{w})}{\partial \mathbf{w} \partial \mathbf{w}^{\mathsf{T}}} = \nabla^2 E(\mathbf{w})$$

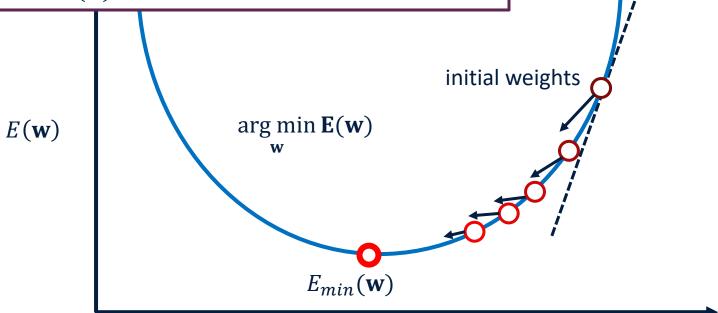
We can use Newton-Raphson

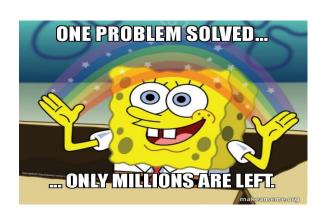
$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \frac{\nabla_{\mathbf{w}_t} E(\mathbf{w}_t)}{\nabla_{\mathbf{w}_t}^2 E(\mathbf{w})}$$

#### **Training a model**, *TL;DR*:

#### **Solution**

• Take repeated small steps t in the direction of steepest decrease of  $E(\mathbf{w})$  ...





#### **Jacobian**

gradient

/gradient

 $\mathbf{W}$ 

$$\mathbf{J} = \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = \nabla E(\mathbf{w})$$

#### Hessian

$$\mathbf{H} = \frac{\partial^{2} E(\mathbf{w})}{\partial \mathbf{w} \partial \mathbf{w}^{\mathsf{T}}} = \nabla^{2} E(\mathbf{w})$$

We can use **Gradient Descent (GD)** 

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \nabla_{\mathbf{w}_t} E(\mathbf{w}_t)$$

Where  $\eta$  is the learning rate,  $\eta > 0$  determining the size of the step

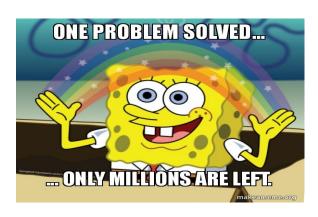
#### **Training a model**, *TL;DR*:

#### **Solution**

- Take repeated small steps t in the direction of steepest decrease of  $E(\mathbf{w})$  ...
- SGD replaces the gradient with an unbiased estimate of the gradient, computing the average gradient over a subset of samples, called a *mini-batch*

 $E(\mathbf{w})$  arg min  $\mathbf{E}(\mathbf{w})$   $\mathbf{E}_{min}(\mathbf{w})$ 

W



#### **Jacobian**

gradient

/gradient

$$\mathbf{J} = \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = \nabla E(\mathbf{w})$$

#### Hessian

$$\mathbf{H} = \frac{\partial^{2} E(\mathbf{w})}{\partial \mathbf{w} \partial \mathbf{w}^{T}} = \nabla^{2} E(\mathbf{w})$$

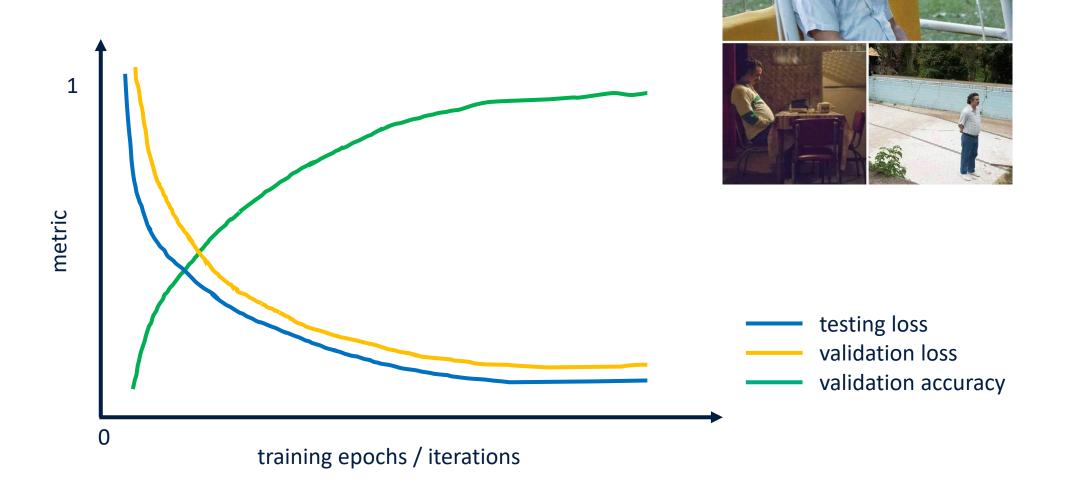
We can use **Stochastic Gradient Descent (SGD)** 

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \frac{1}{m} \nabla_{\mathbf{w}_t} \sum_{i=1}^m E(\mathbf{w}_t)$$

Where  $\eta$  is the learning rate,  $\eta > 0$  determining the size of the step

#### Training a model, TL;DR:

## How to train your model



Waiting on your model to train

### Avoiding Overfitting

#### Tips:

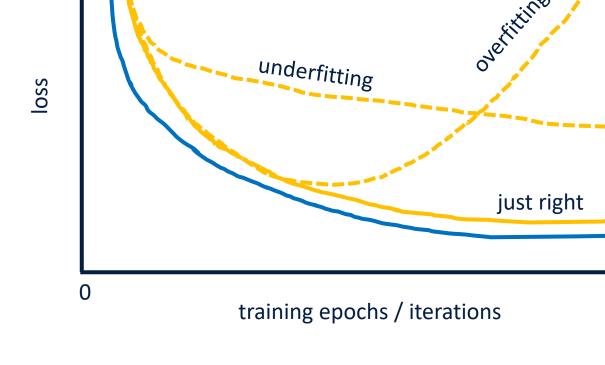
1) adjust your learning rate

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \frac{1}{m} \nabla_{\mathbf{w}_t} \sum_{i=1}^m E(\mathbf{w}_t)$$

Where  $\eta$  is the learning rate,  $\eta>0$  determining the size of the step

- 2) Add regularization by penalizing your loss function
- 3) Add dropout to your model

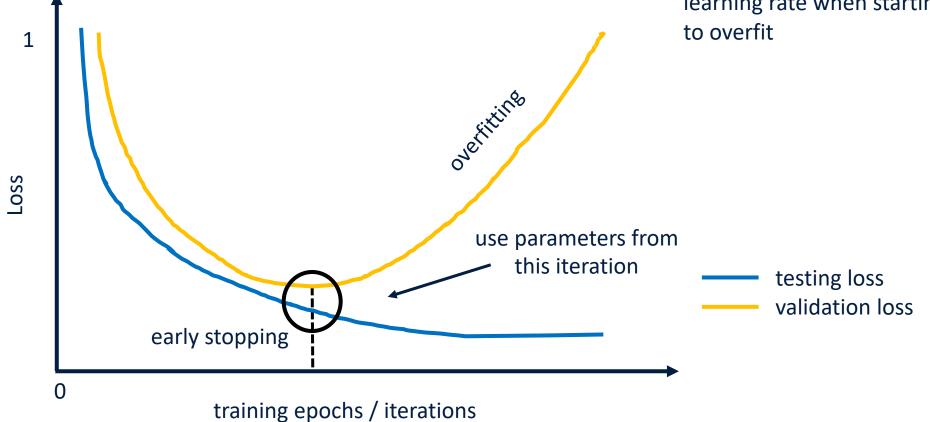
testing lossvalidation loss

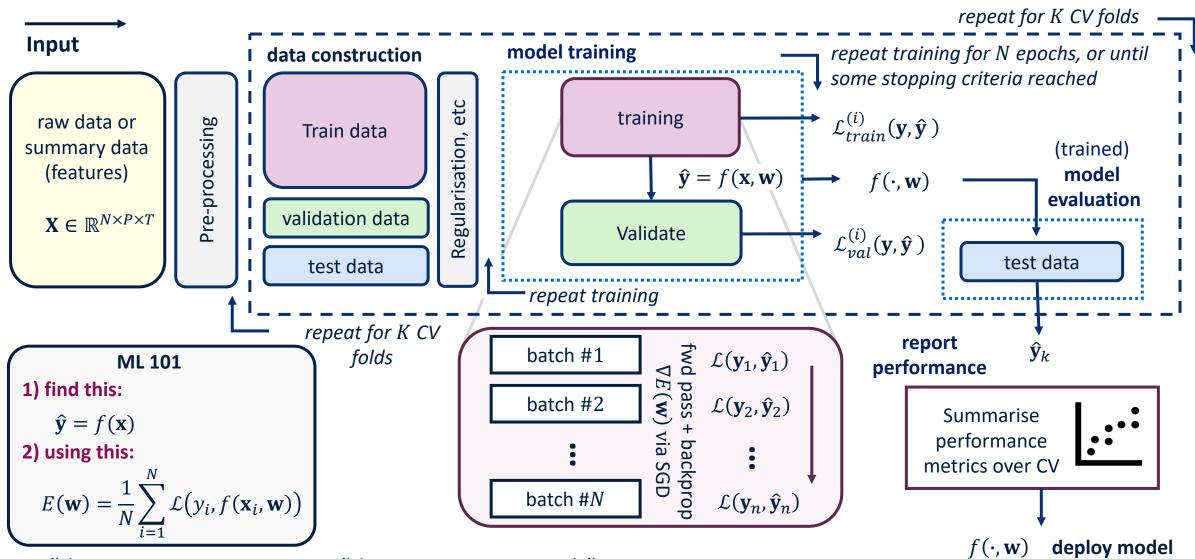


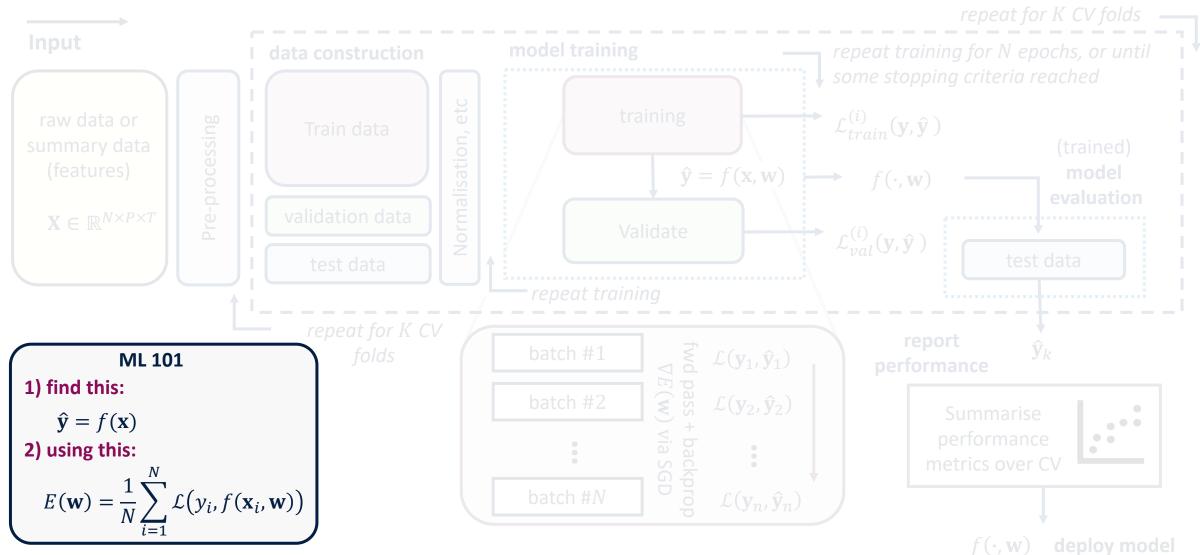
## Avoiding Overfitting

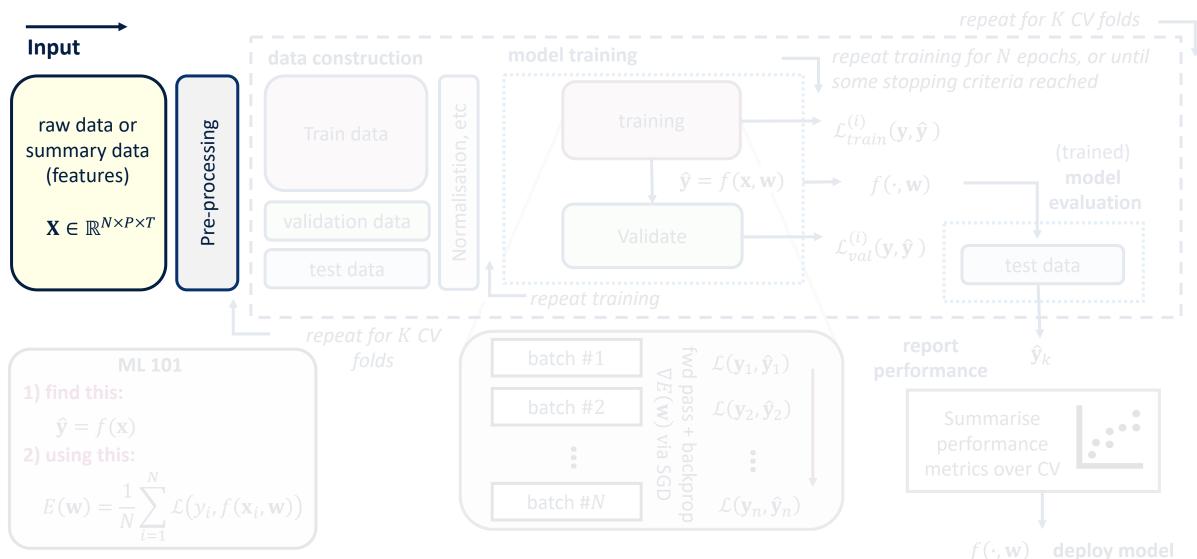
#### Tips:

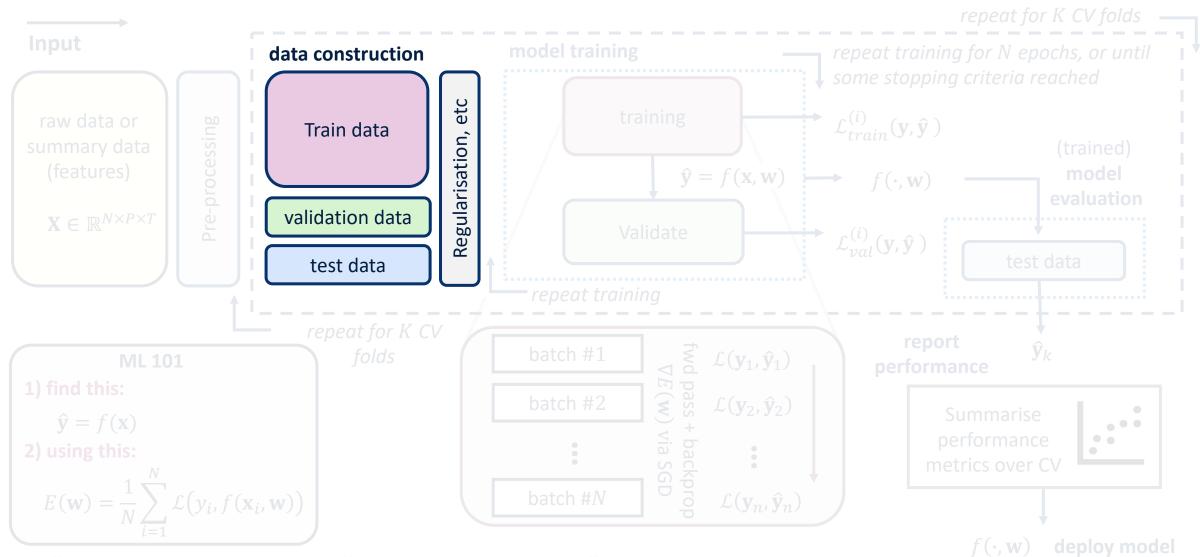
- 4) Add early stopping criteria
- 5) Dynamically lower your learning rate when starting

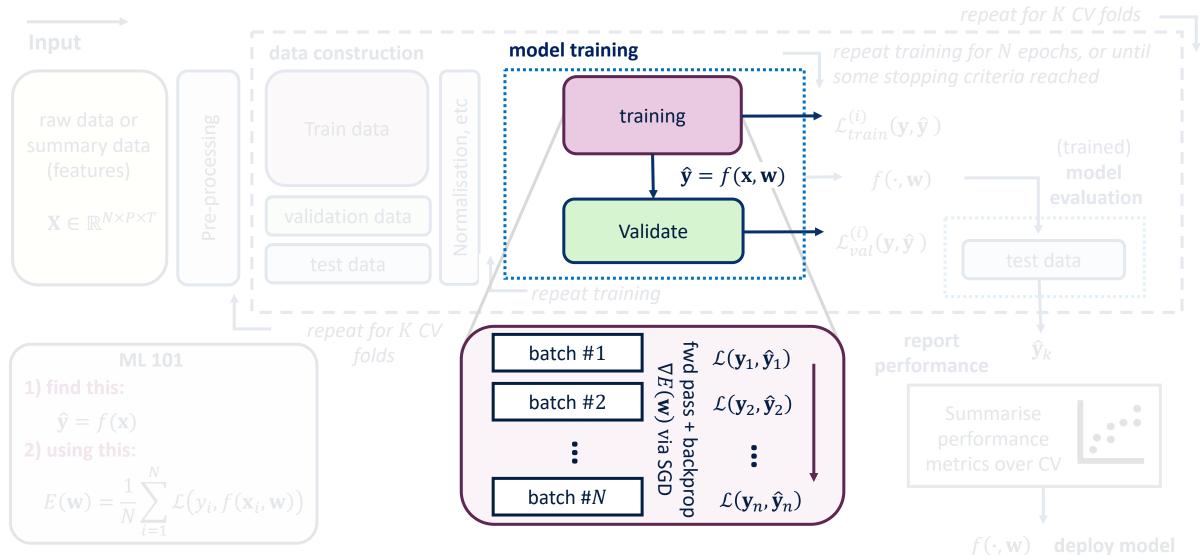


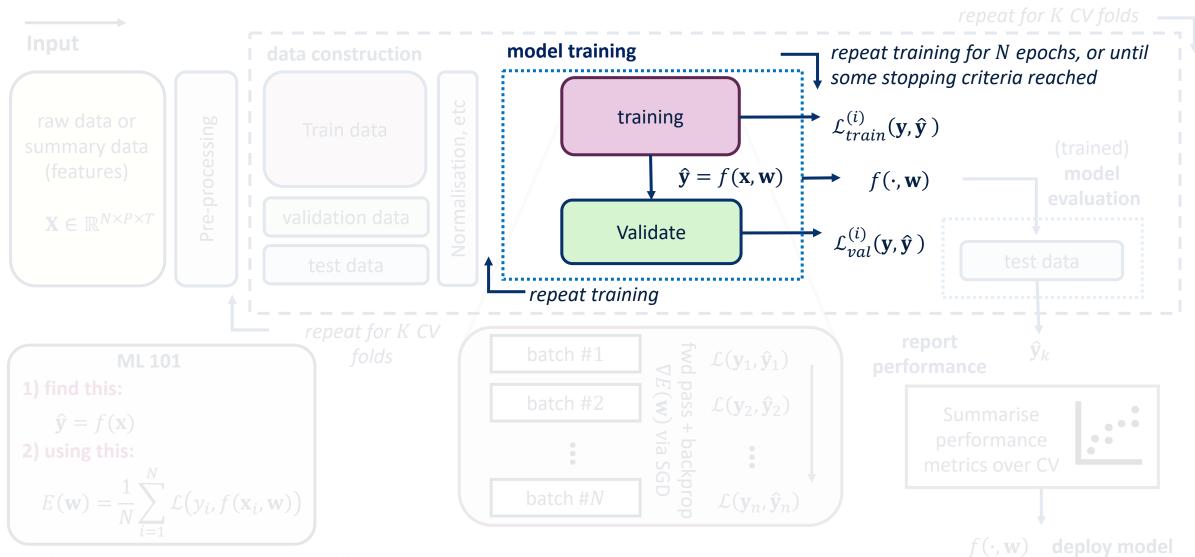


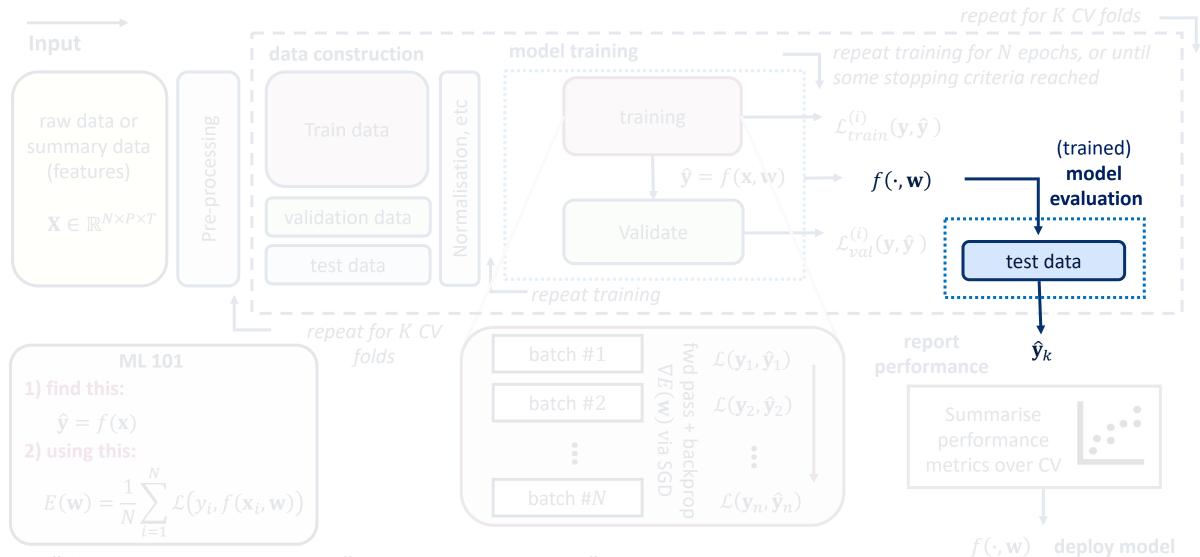


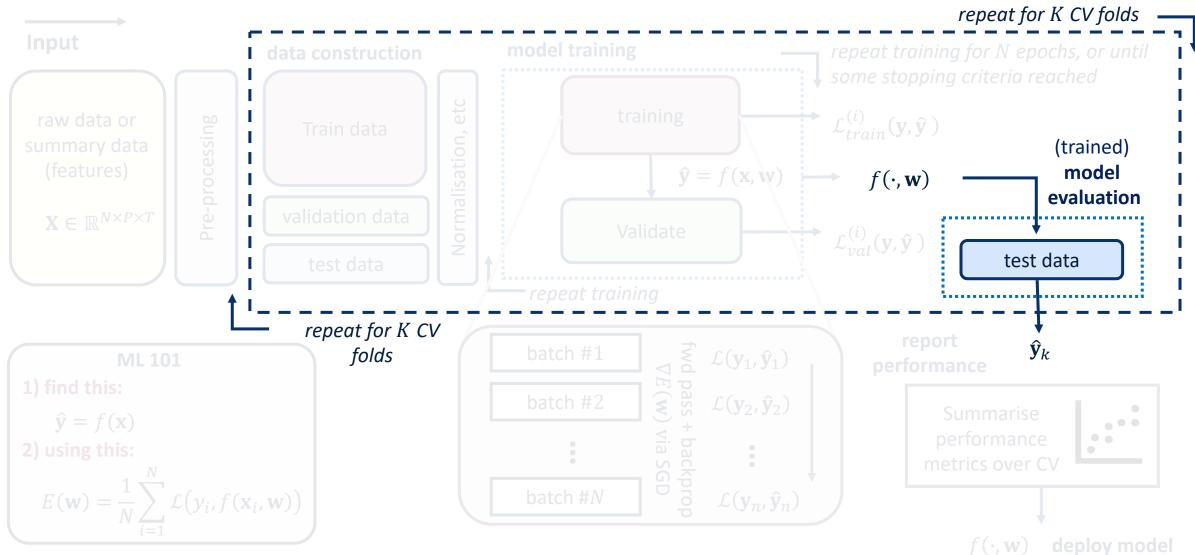


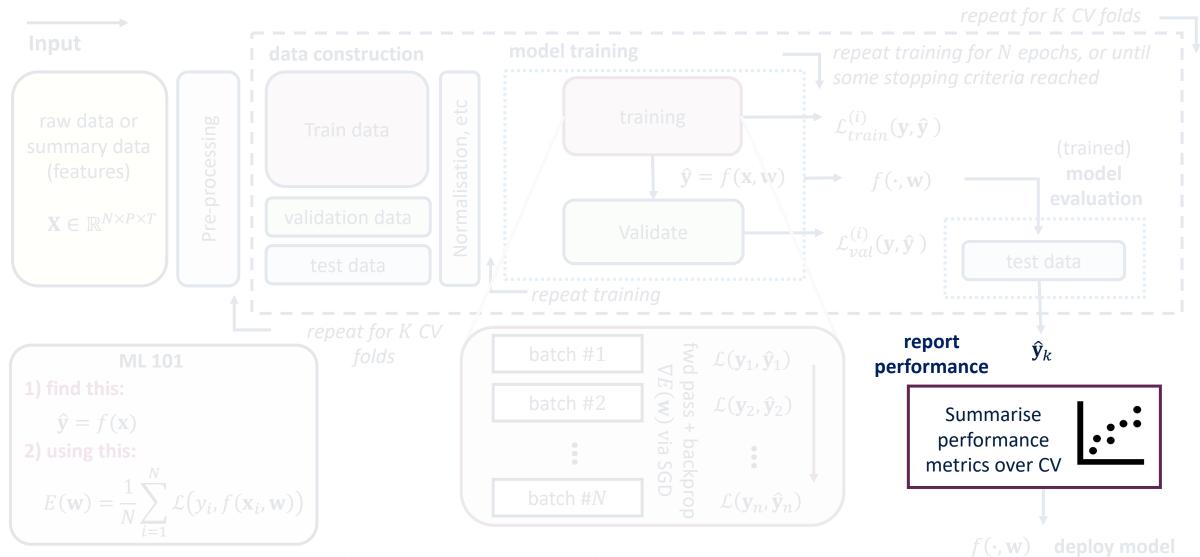


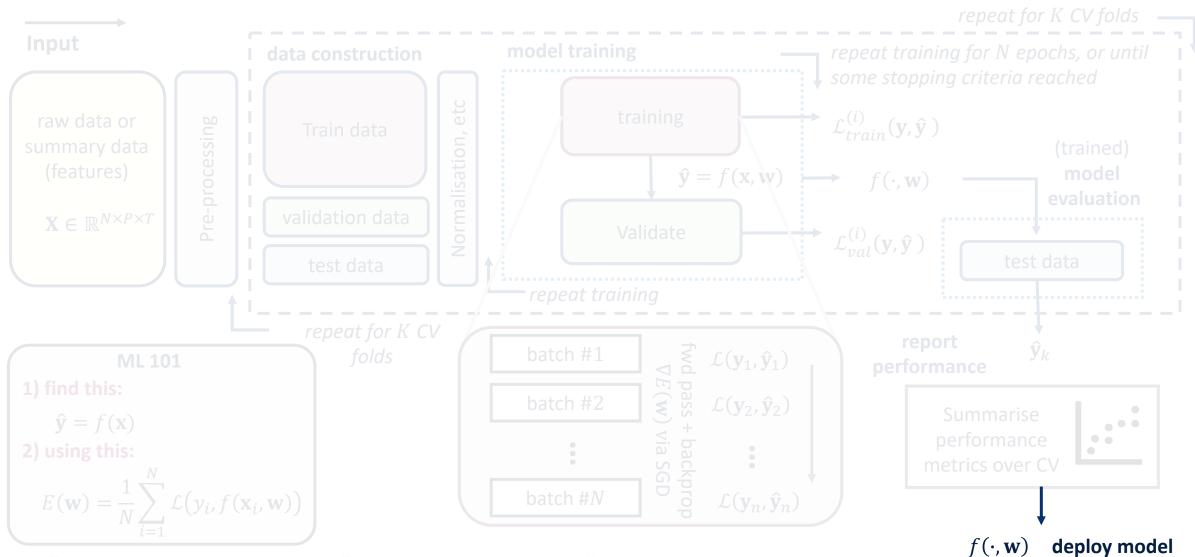


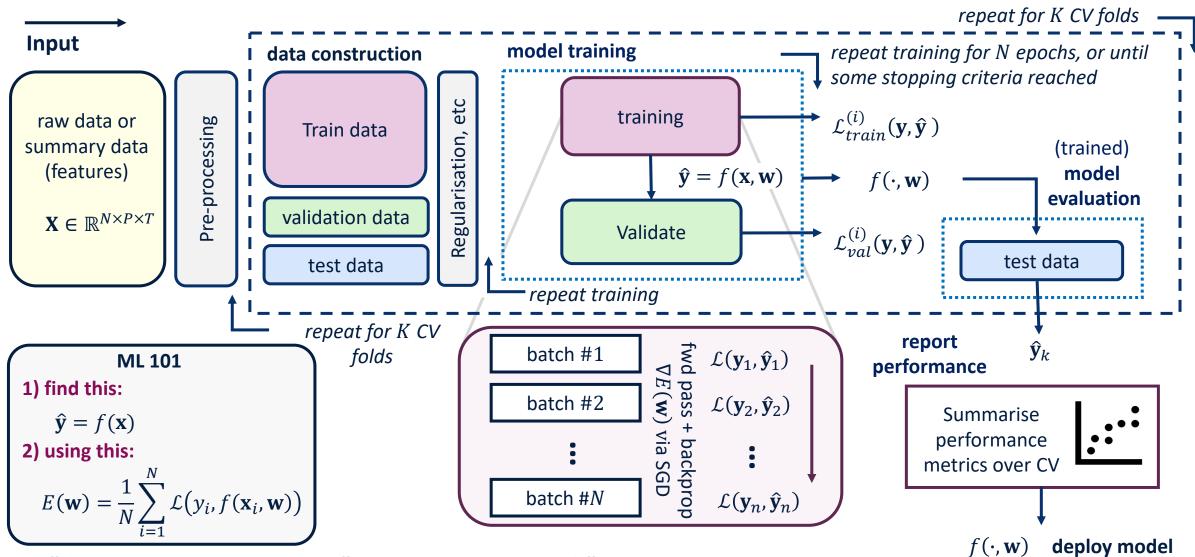














### ML 4 Time-series: Recurrent Neural Networks

What have we learned?

- Assuming individual time-steps as I.I.D. is a naïve approach
- Incorporating recurrence into our networks can model temporality
- RNNs are prone to vanishing and exploding gradient problems
- Gated cells, such as LSTMS overcome these difficulties, allowing us to model longterm dependencies
- How we can implement and train RNNs/LSTMS
- What a typical machine learning pipeline should look like