Time Series Modeling using Neural Networks

Dušan Fedorčák

11/2021 – RBI

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Background

- Ph.D. in computer science at VŠB-TU Ostrava
  - Neural networks & unsupervised self-organization
- Experienced in simulations
  - flood prediction system for MSK
  - traffic monitoring & prediction systems
- Experienced in computer graphics & scientific visualization
  - GIS related real-time 3D visualizations
- 5+ years in applied ML and artificial intelligence
  - Lead researcher in GoodAI – general artificial intelligence
  - CTO in Neuron Soundware – sound processing via Deep Learning
  - Lead ML in Merlon Intelligence Inc. – natural language processing

Content

DAY 1

- **Classical time series analysis**
  - *Decomposition of time series*
  - *ARIMA models family*
  - *State space models generalization*
- **Theoretical window**
  - *Neural Networks & Recurrent NNs*
  - *Time series specifics*
- **Practical examples**
  - *Simple regression – toy example*
  - *Rainfall-runoff simulation – regression*

– lunch break –

- **Practical examples**
  - *Trampoline jumping – classification*
  - *Local Weather Forecast – regression*

DAY 2

- **Product Design & ML**
  - *Integration of ML models into products*
  - *Tips & tricks for debuging NNs*
- **Practical Examples** (in random order)
  - *Exoplanets Hunting*
  - *Mobile Motion Sensing*

– lunch break –

  - *Manufacturing Process Modeling*
  - *Financial distress prediction*

- *Google Drive Folder with data*
- *GitHub repository with example sources*

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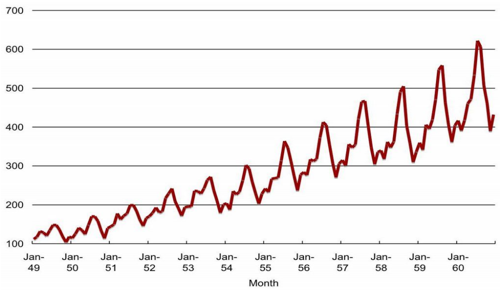
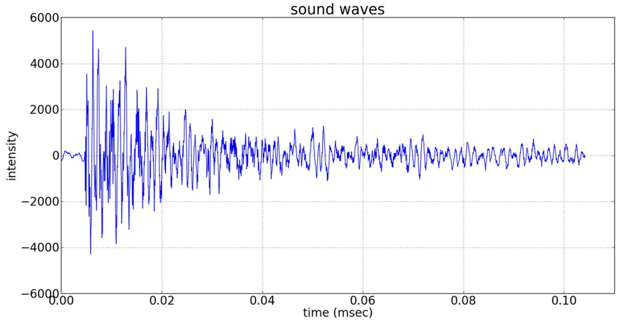
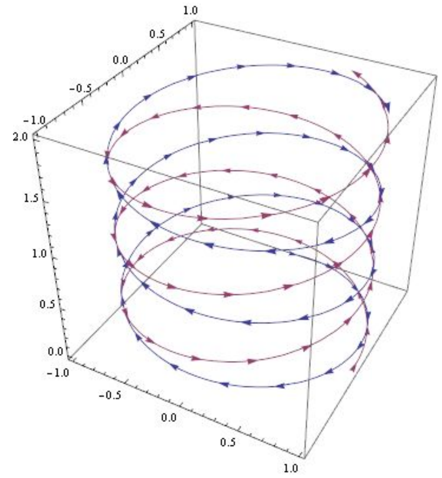
Time series – example data







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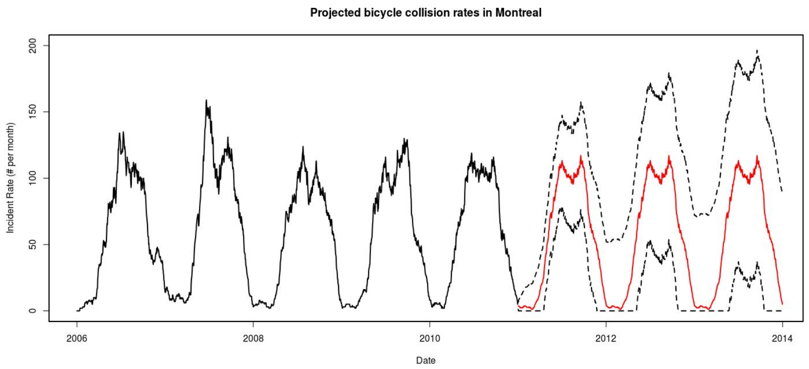
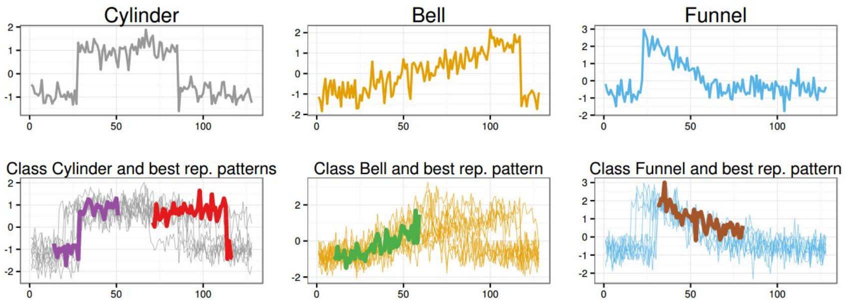
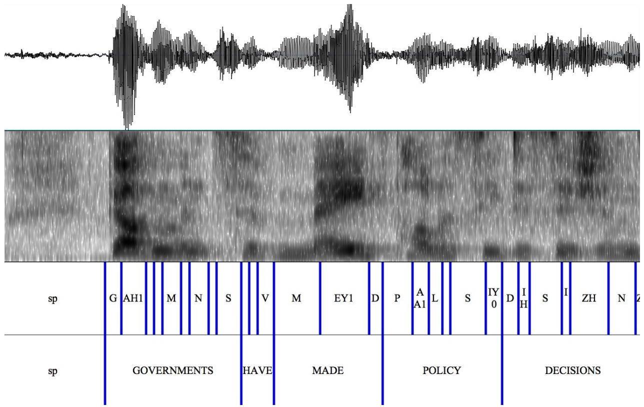
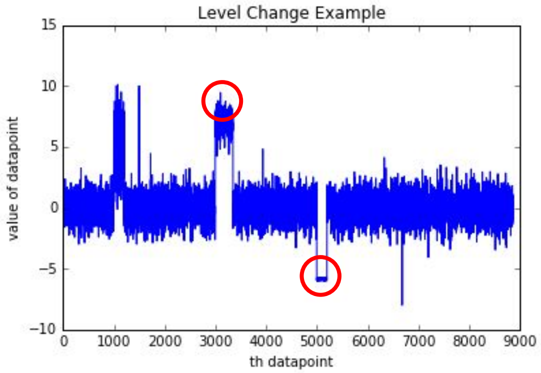
Time series – example tasks









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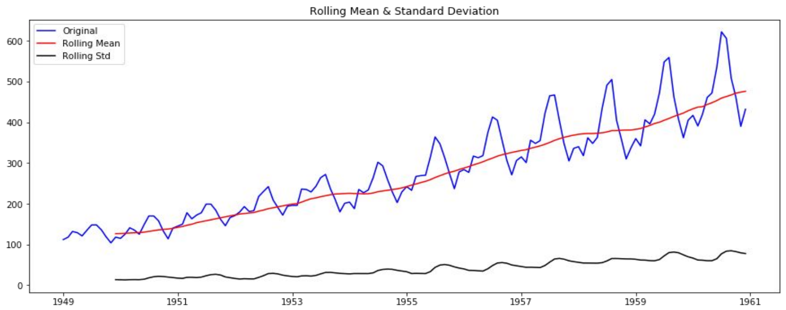
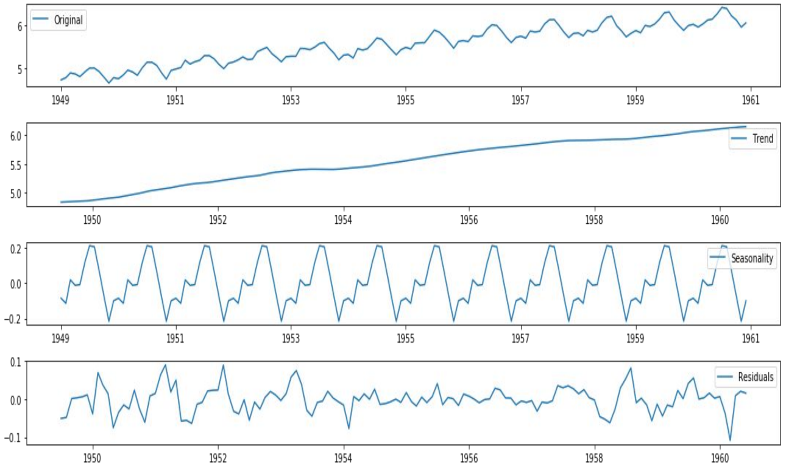
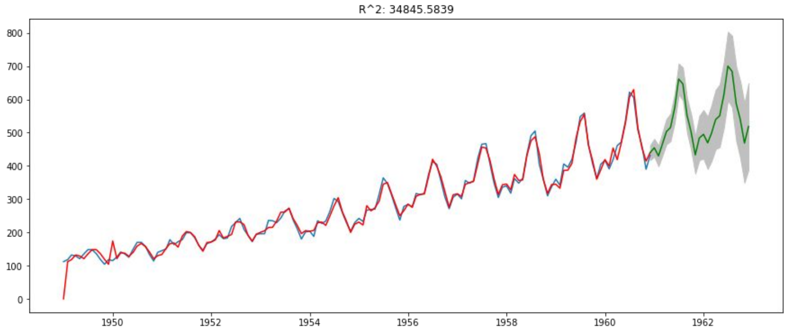
Time Series – classical analysis & modeling

- Time Series Decomposition
  - Inflation, trend, seasonality, differencing
- ARIMA models
  - http://people.duke.edu/~rnau/411home.htm







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State Space Models

- State Space Models
  - A dynamic system that **evolves over time**
  - Knowing **the current state of the model is enough** to predict the future
  - The true state of the system might **not** be **directly observable**
- Model Description
  - State
    - $\boldsymbol{x}_t \sim N(\boldsymbol{x}_t, \boldsymbol{P}_t)$
  - State Equation
    - $\boldsymbol{x}_t = \boldsymbol{F}\boldsymbol{x}_{t-1} + N(0, \boldsymbol{Q})$ – *sometimes without noise*
  - Observation Equation
    - $\boldsymbol{y}_t = \boldsymbol{H}\boldsymbol{x}_t + N(0, \boldsymbol{R})$

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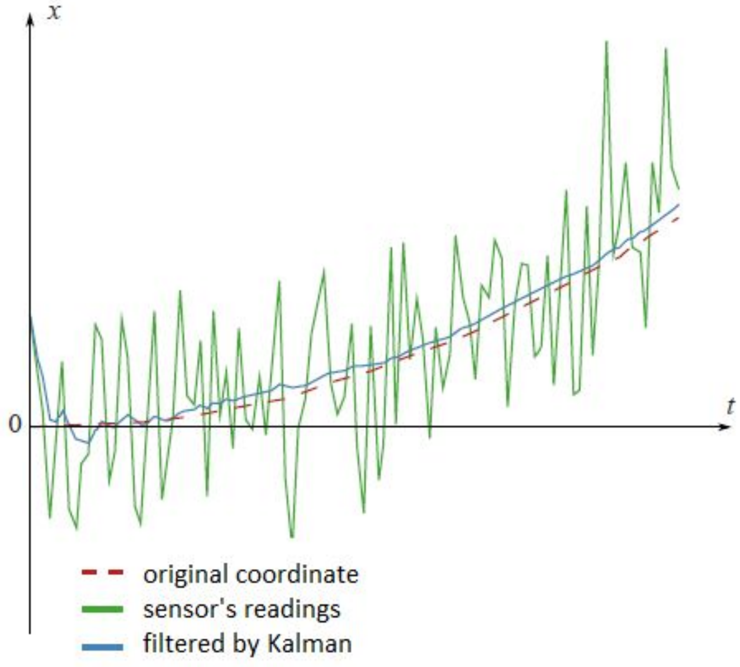
Kalman Filter

- Evolve state
  - $x'_t = Fx_{t-1}$
  - $P'_t = F\,P_{t-1}F^T + Q$
- Integrate observation
  - $x_t = x'_t + K_t(y_t - Hx'_t)$
  - $P_t = (I - K_tH)\,P'_t$
- **Kalman Gain**
  - $K_t = P'_t\,H^T(HP'_tH^T + R)^{-1}$
- ARIMA and Kalman Filter
  - ARIMA can be viewed as a state space model
  - ARIMA can be fitted with MLE via Kalman Filter
  - https://bookdown.org/rdpeng/timeseriesbook/maximum-likelihood-with-the-kalman-filter.html
  - https://towardsdatascience.com/the-kalman-filter-and-maximum-likelihood-9861666f6742



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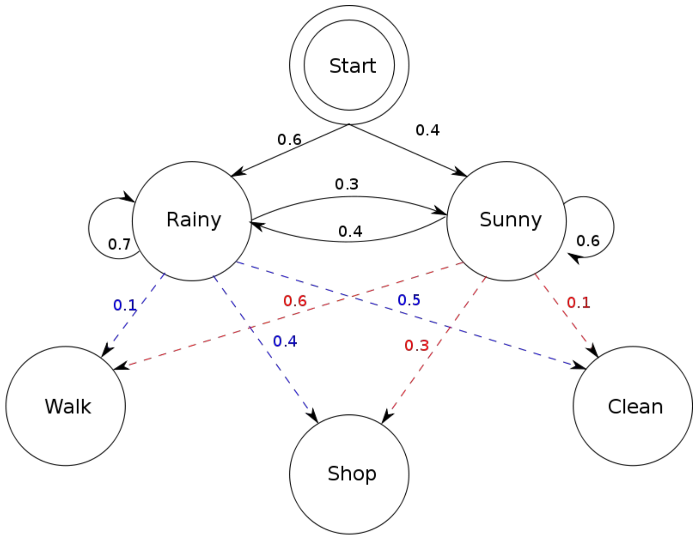
Hidden Markov Model

- Model Description
  - HMM ($\boldsymbol{\lambda}$) can be viewed as a **state space model**
  - Finite set of hidden states
    - $\mathbf{Q} = \{q_1, q_2, \dots, q_n\}$, $\boldsymbol{\pi} = \{\pi_1, \pi_2, \dots, \pi_n\}$ – init
    - $\boldsymbol{n}$ – number of states (hyperparameter)
  - Set of observations
    - $\mathbf{O}_i = (o^1, o^2, o^3, \dots, o^T)$
  - Transition probability matrix & emissions
    - $\boldsymbol{A} = (a_{00}, \dots, a_{nn})$, $\mathbf{B} = q_i \to o$



- Model Capabilities
  - $P(\mathbf{O}|\boldsymbol{\lambda})$ – Give prob. of **O** being produced by $\boldsymbol{\lambda}$ – *forward-backward alg.*
  - $P(\mathbf{q}_1, \dots, \mathbf{q}_t|\mathbf{O}, \boldsymbol{\lambda})$ – Give most likely sequence of states for given **O** – *Viterbi alg.*
  - $\mathbf{O} \Rightarrow \boldsymbol{\lambda}$ – Model must be trainable with **O** – *Baum-Welch alg.*

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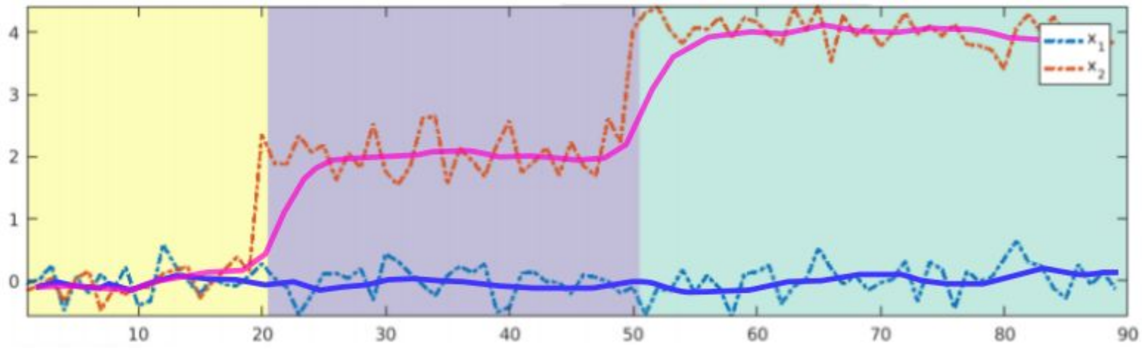
Kalman Filter vs. Hidden Markov Model

- **Kalman Filter**
  - Continuous state
  - Generic state & observation equation
  - Linear dynamic system
  - *Fusion of sensor readings and controls*
  - *ARMA models implementation*
- **Hidden Markov Model**
  - Discrete set of states
  - N-states hyperparameter
  - Emission & Transition tables
  - *Speech recognition*
  - *Time series segmentation*



http://lasa.epfl.ch/teaching/lectures/ML_MSc_Advanced/Slides/Lec_XI_HMM_extensions.pdf

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Time Series – goal in classical terminology

- **Forecasting**
  - Given the past and the present observation, what will the future look like?
- **Time scale analysis**
  - Given the observations, what time scales dominate when observing temporal variation in the data
- **Filtering**
  - Given the past and the present observation, how should I update my estimate of the true state of nature?
- **Smoothing**
  - Given a complete dataset, what can I infer about the true state of nature in the past?
- **Regression**
  - Given a time series of two phenomena, what is the association between them?

https://bookdown.org/rdpeng/timeseriesbook/

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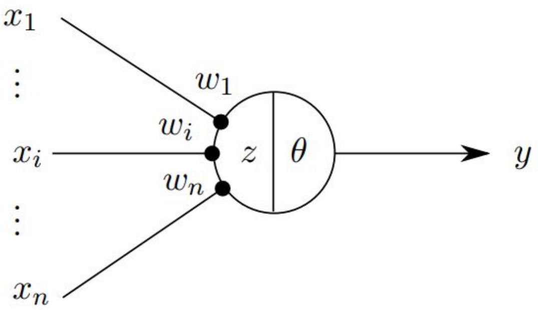
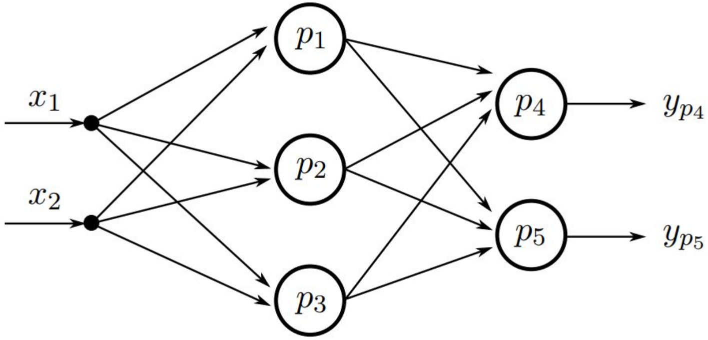
Neural networks





- Artificial Neural Cells
  - Linear combination of inputs
  - Non-linear activation function
- Connected Neurons
  - Directed graph
  - Layered structure
    - Dense connections
    - Convolutions & pooling
    - Recurrency, signal gates
    - Masking & attention heads
- Universal function approximator
  - Trainable with data
  - Backpropagation
  - Deep vs. shallow architecture

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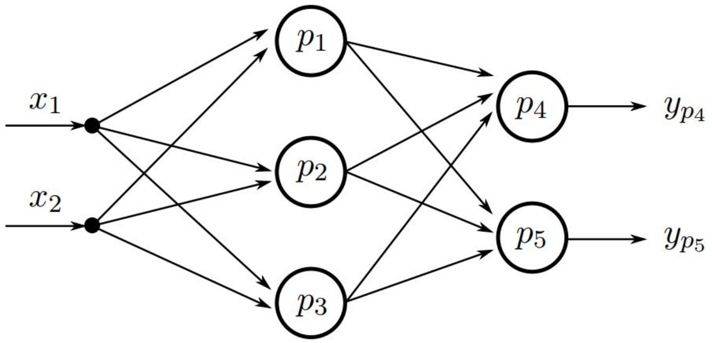
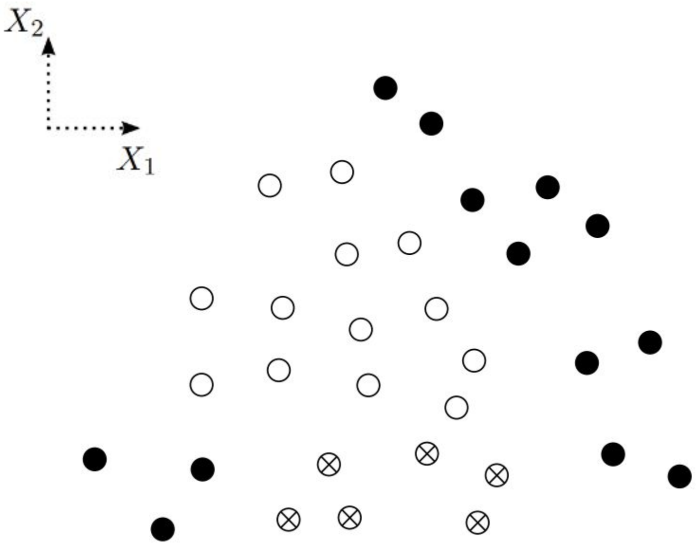
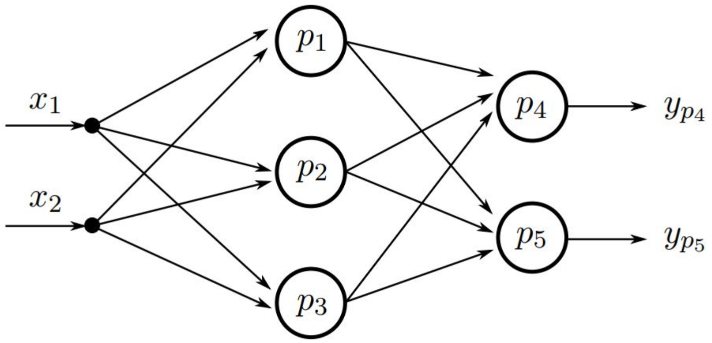
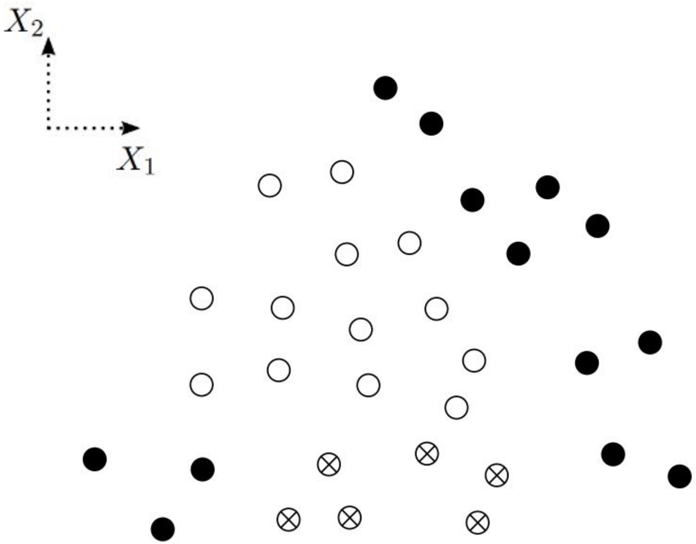
Neural networks – Input space separation





Neural networks – Input space separation





$$y = s(\Sigma\, w_i x_i - \theta)$$

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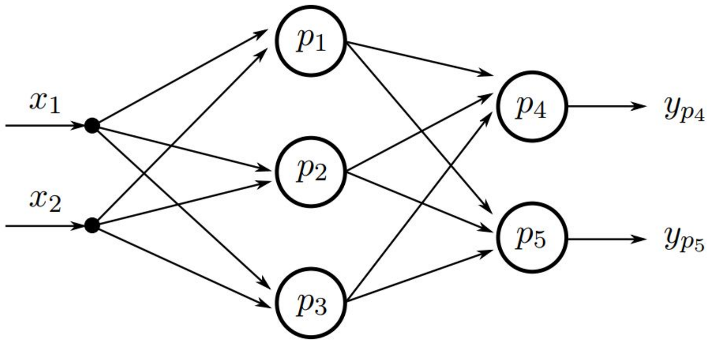
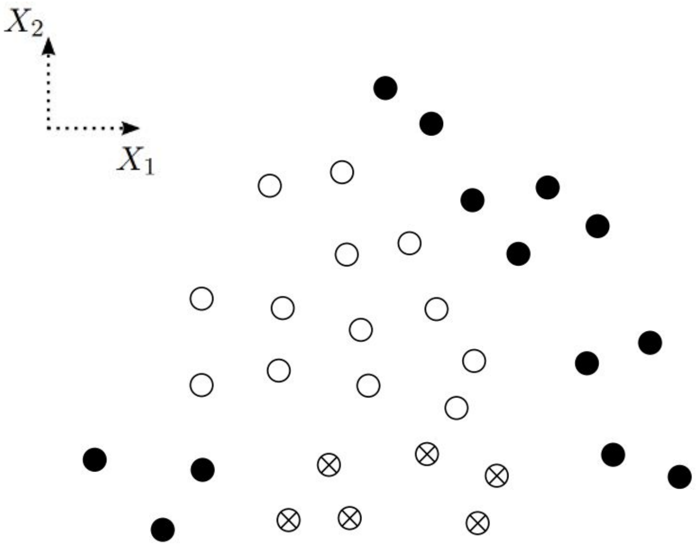
Neural networks – Input space separation





$$y = s(\Sigma\, w_i x_i - \theta) = s(w_1 x_1 + w_2 x_2 - \theta)$$

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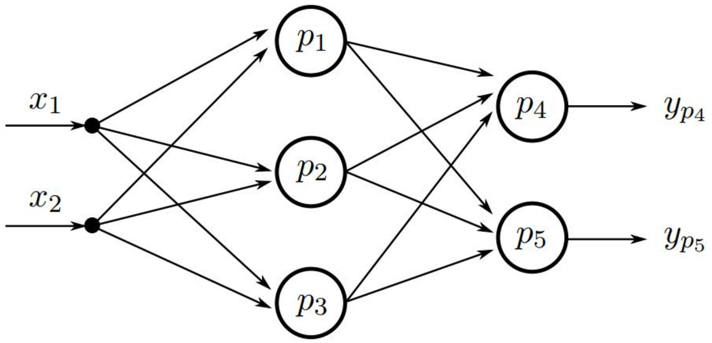
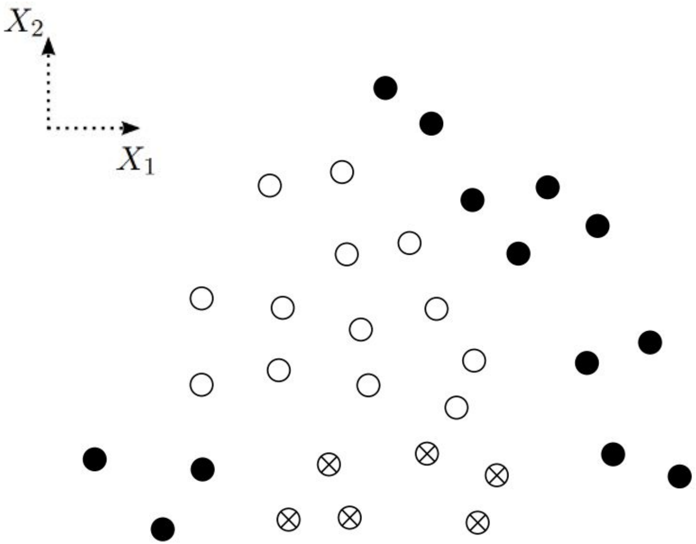
Neural networks – Input space separation





$$ax + by + c = 0$$

$$y = s(\Sigma w_i x_i - \theta) = s(w_1 x_1 + w_2 x_2 - \theta)$$

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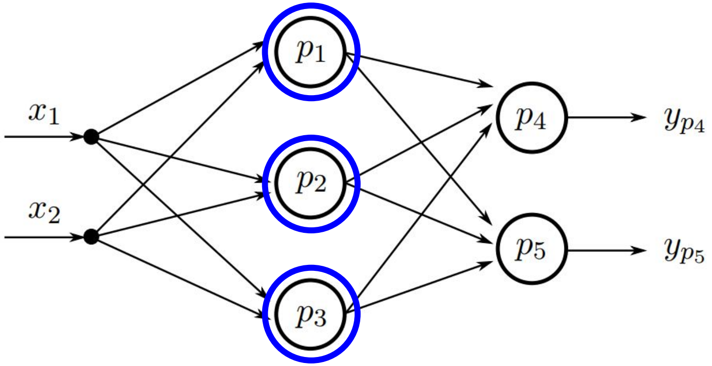
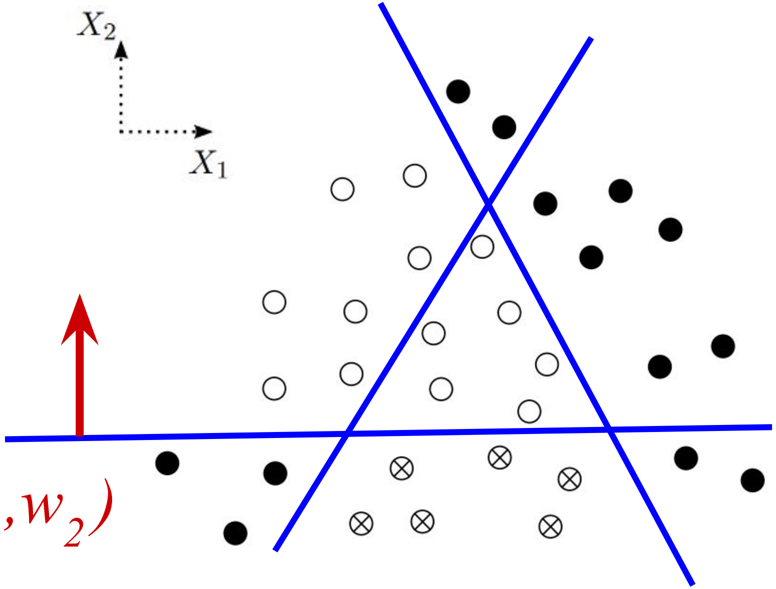
Neural networks – Input space separation



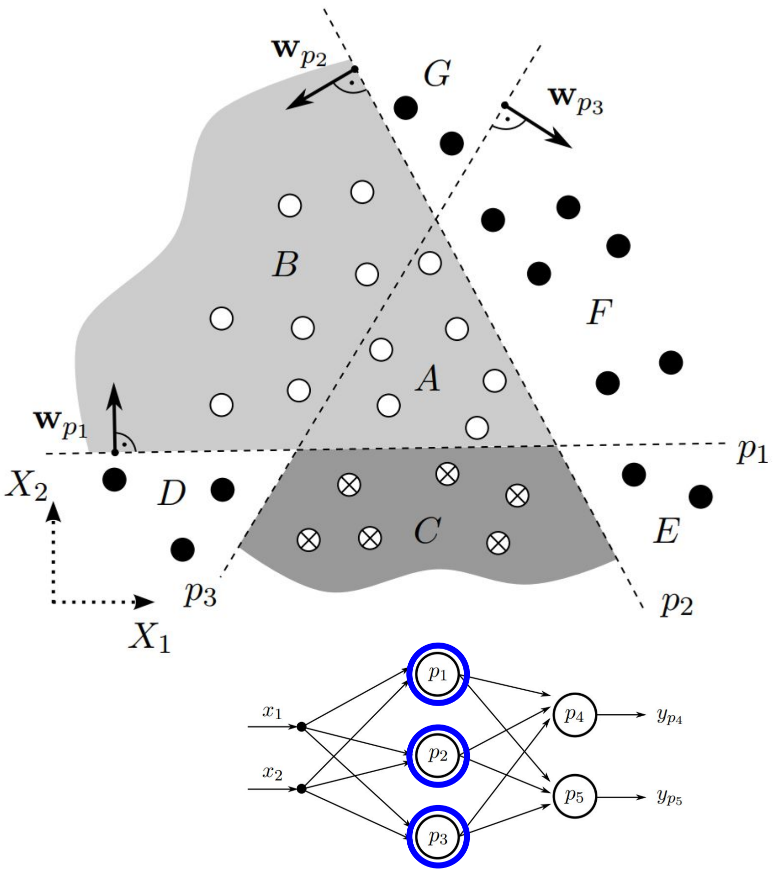


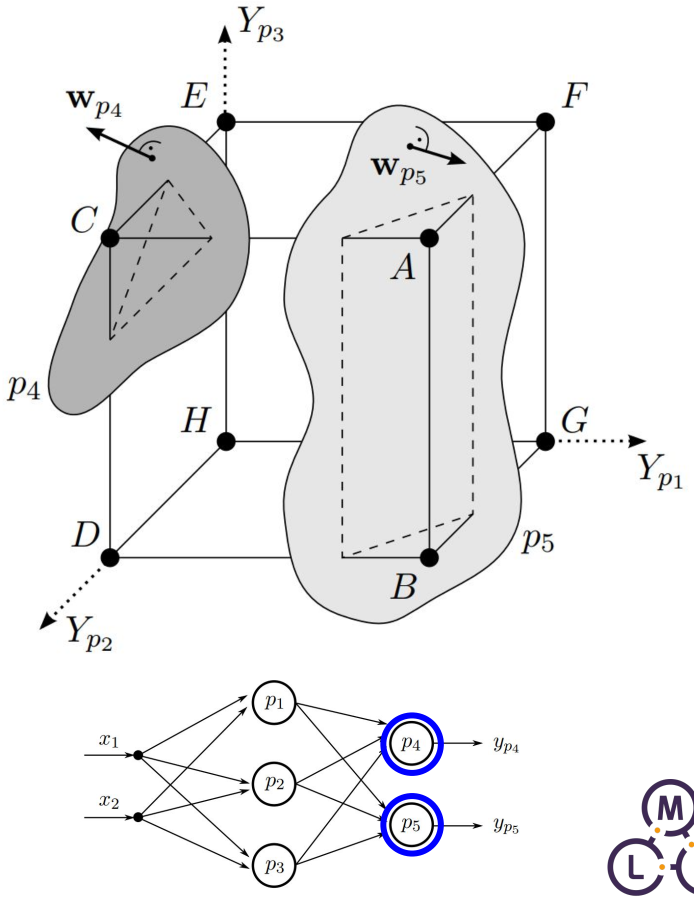
$$(a,b) = (w_1, w_2)$$

$$ax + by + c = 0$$

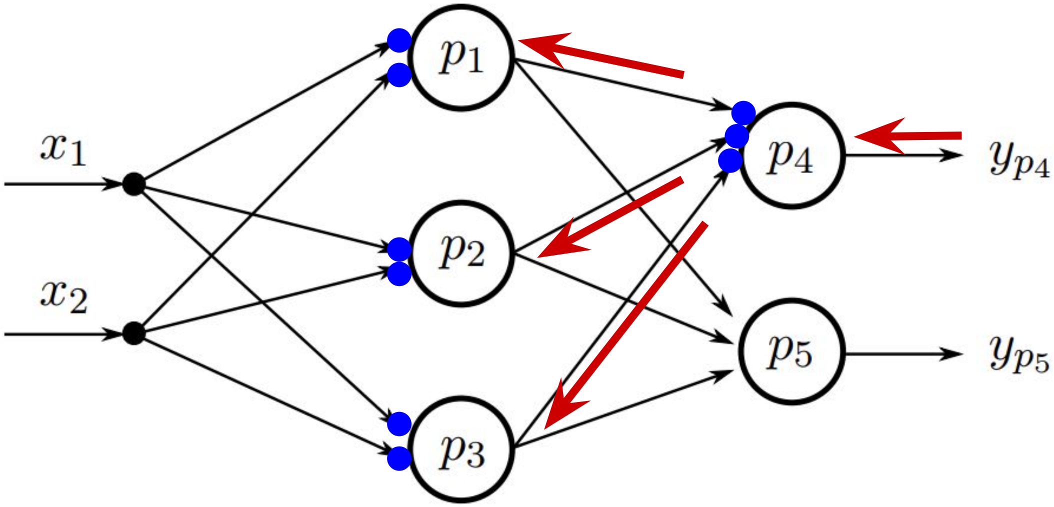
$$y = s(\Sigma\, w_i x_i - \theta) = s(w_1 x_1 + w_2 x_2 - \theta)$$

Neural networks – Input space separation

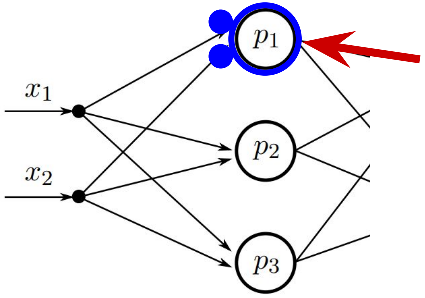


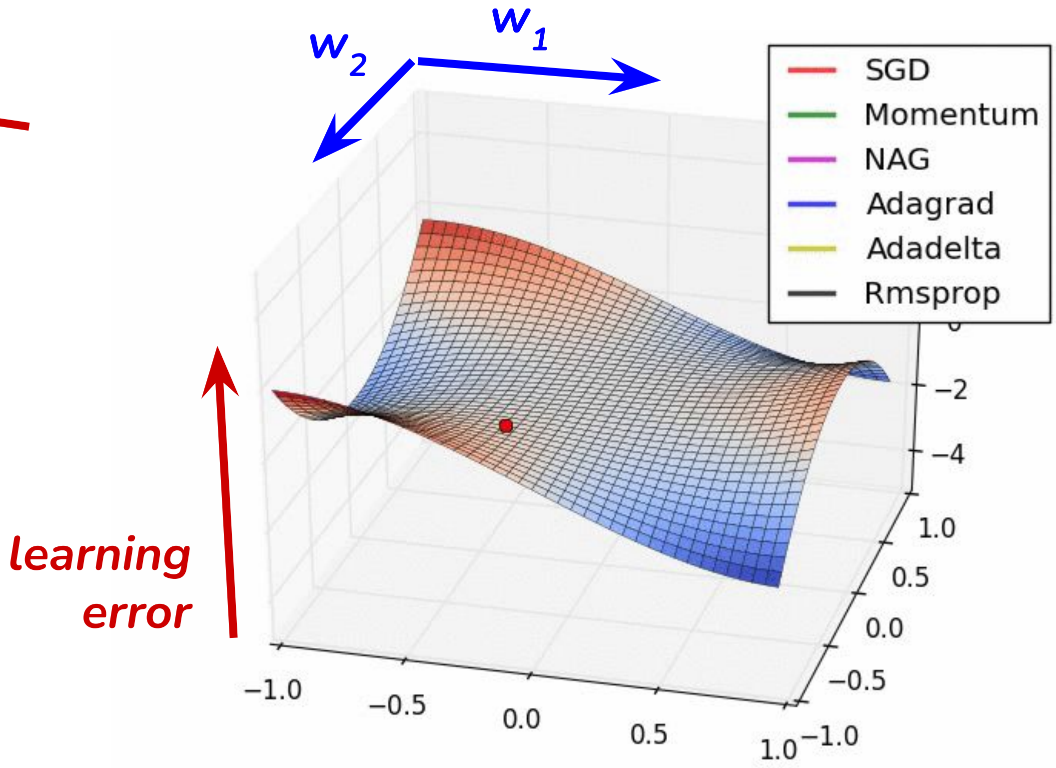


Neural networks – Backpropagation



Neural networks - Backpropagation





http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html

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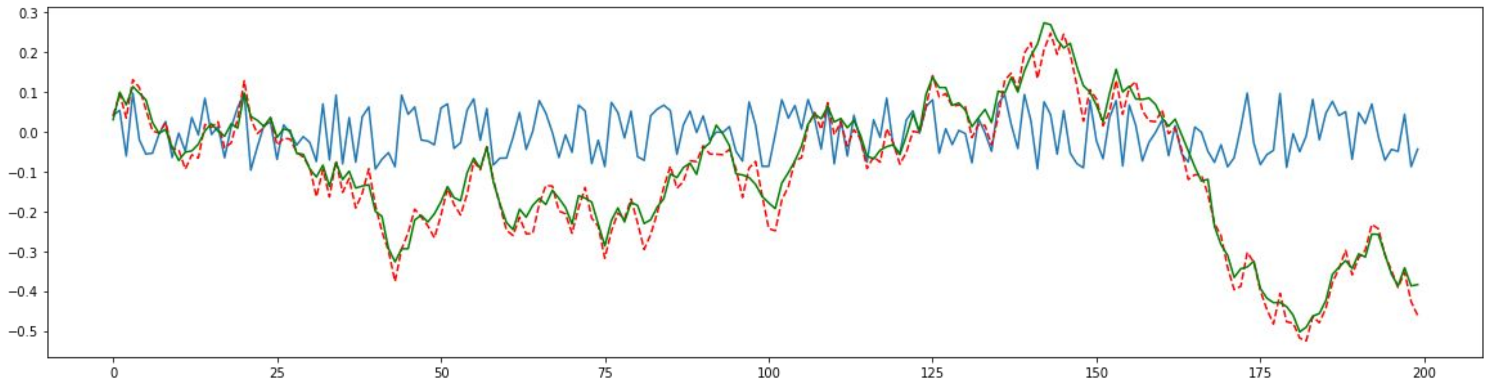
Time Series with Neural Networks



- Neural Networks
  - How to **express time domain**
  - How to **prepare training data**
  - How to **design the model**
  - How to **train & test the model**

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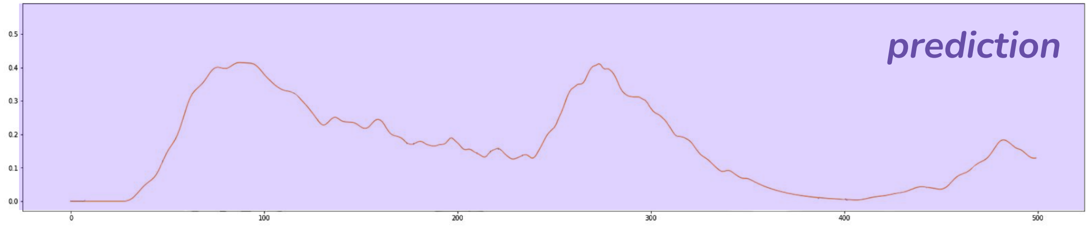
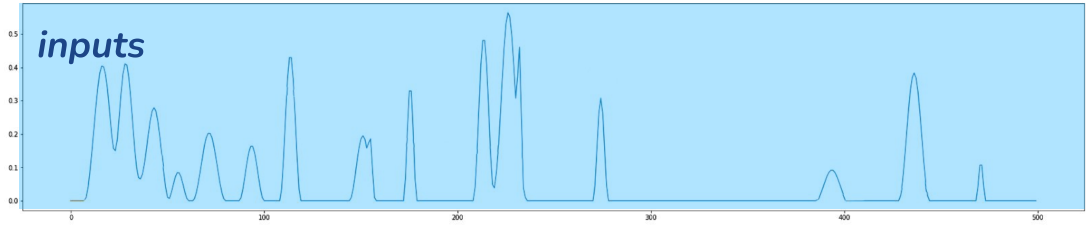
How neural network fits?





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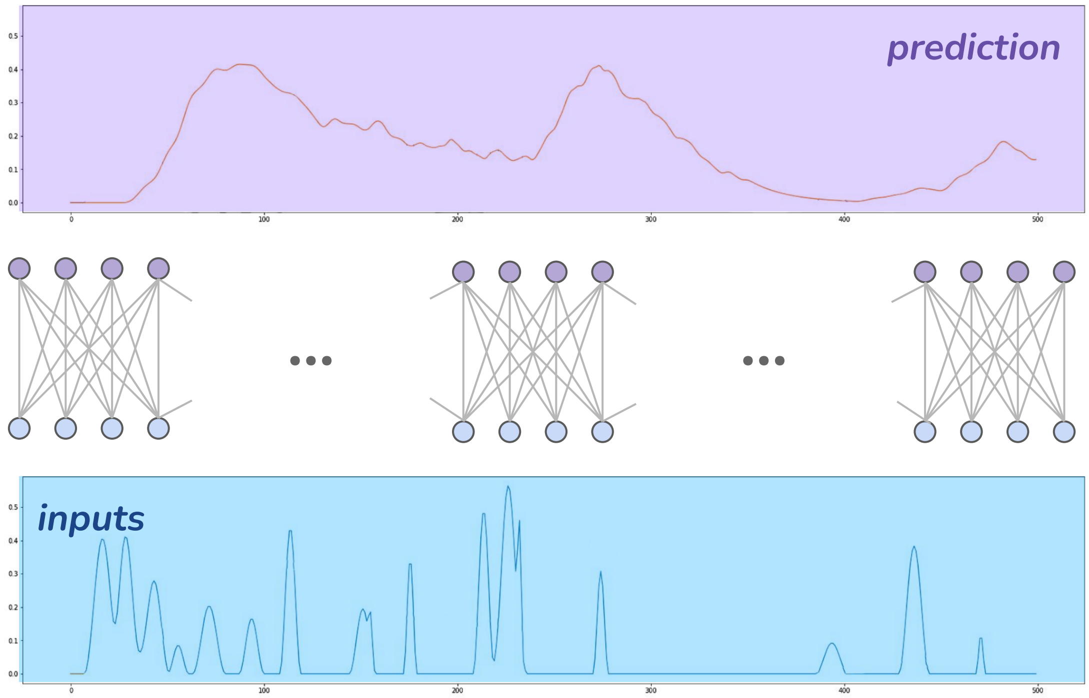
Simple feed-forward network



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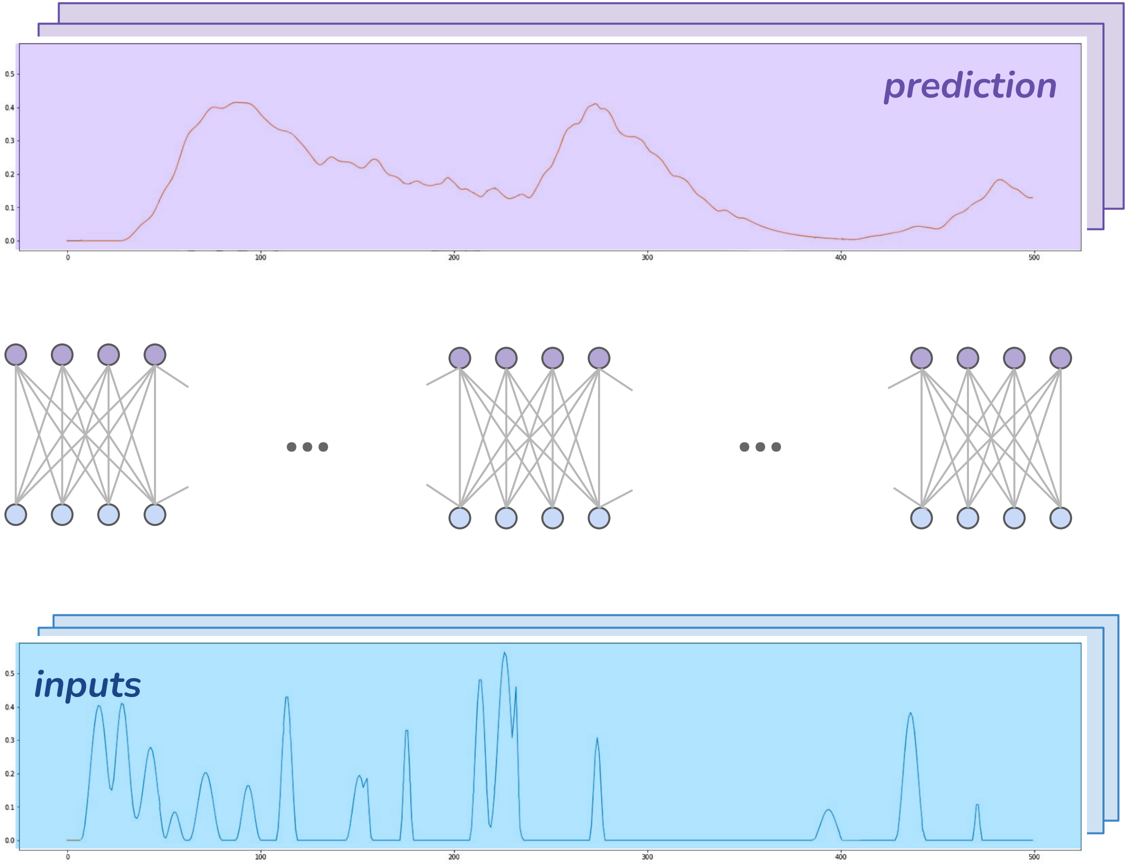

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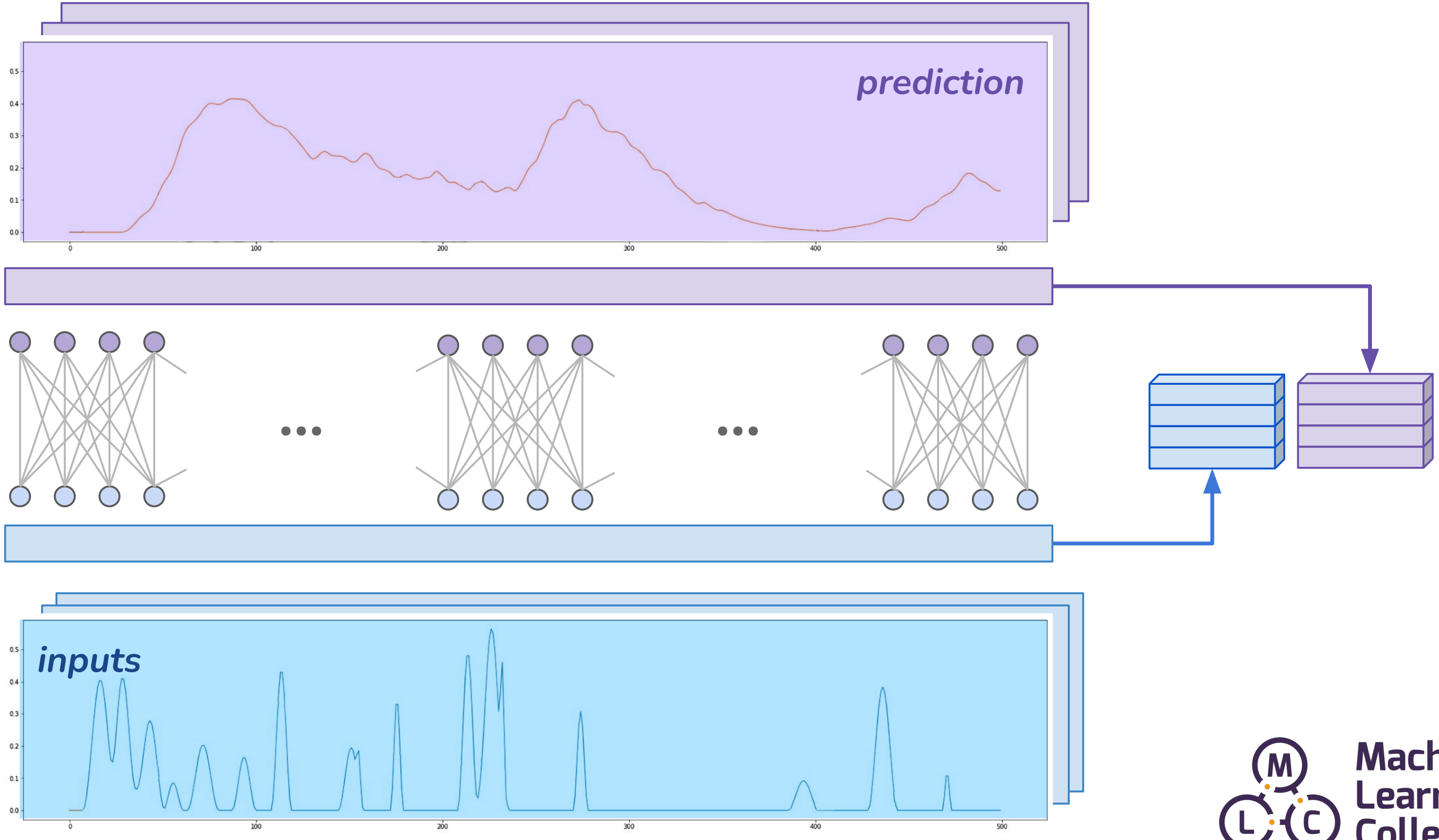

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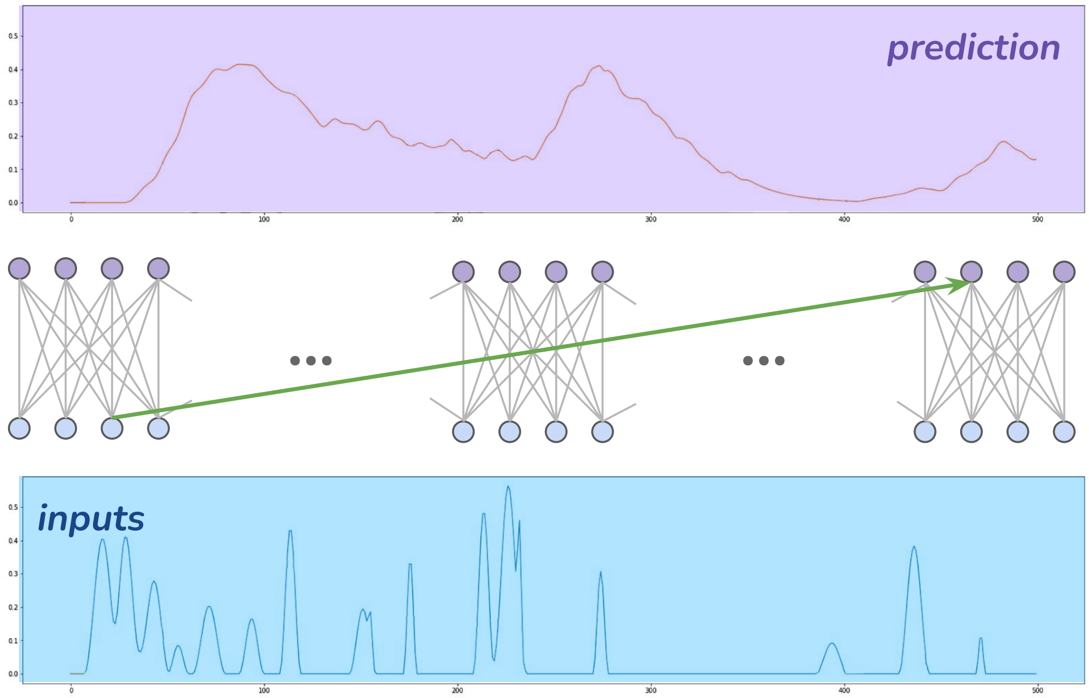

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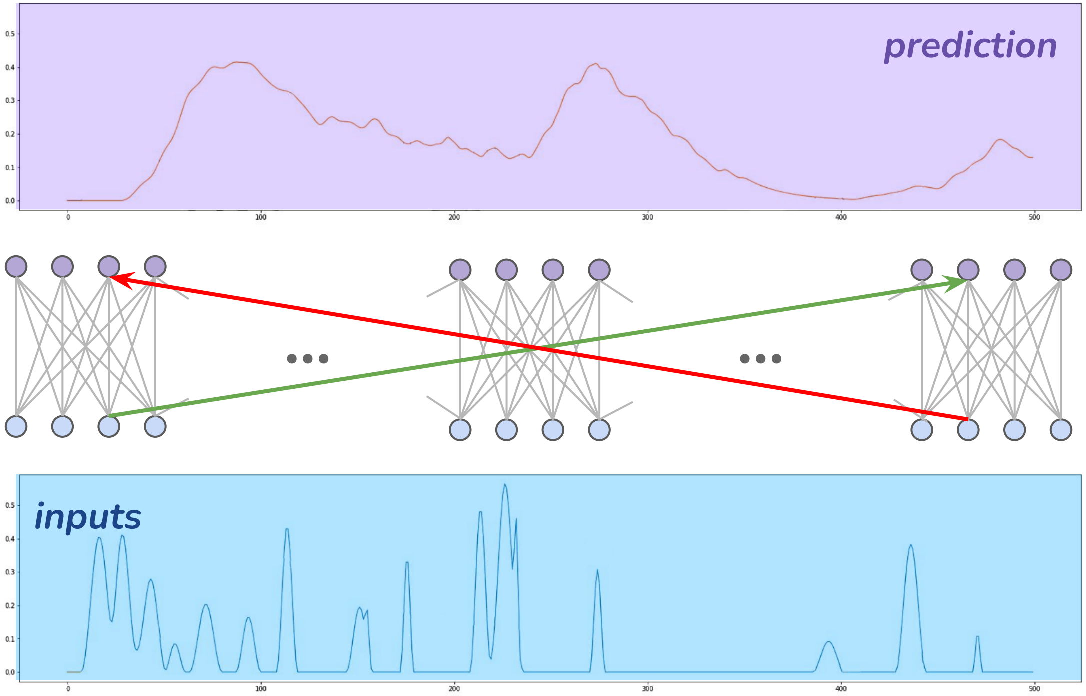

predicting
from future ?

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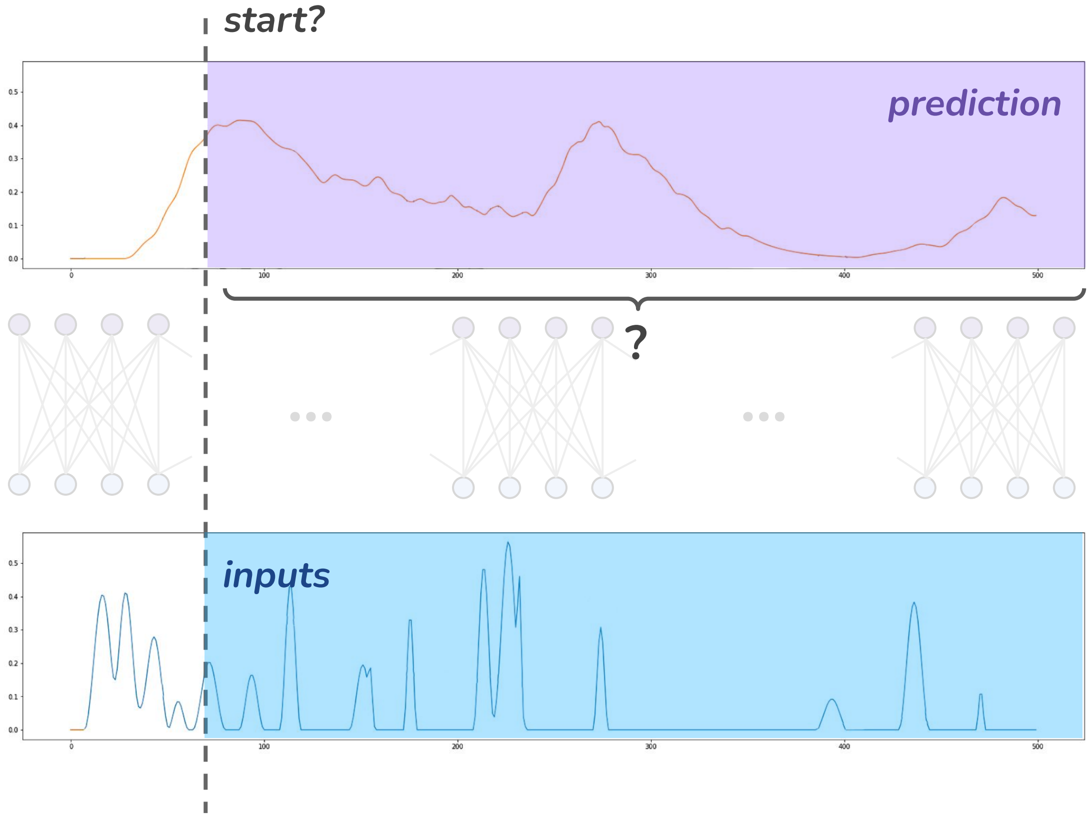
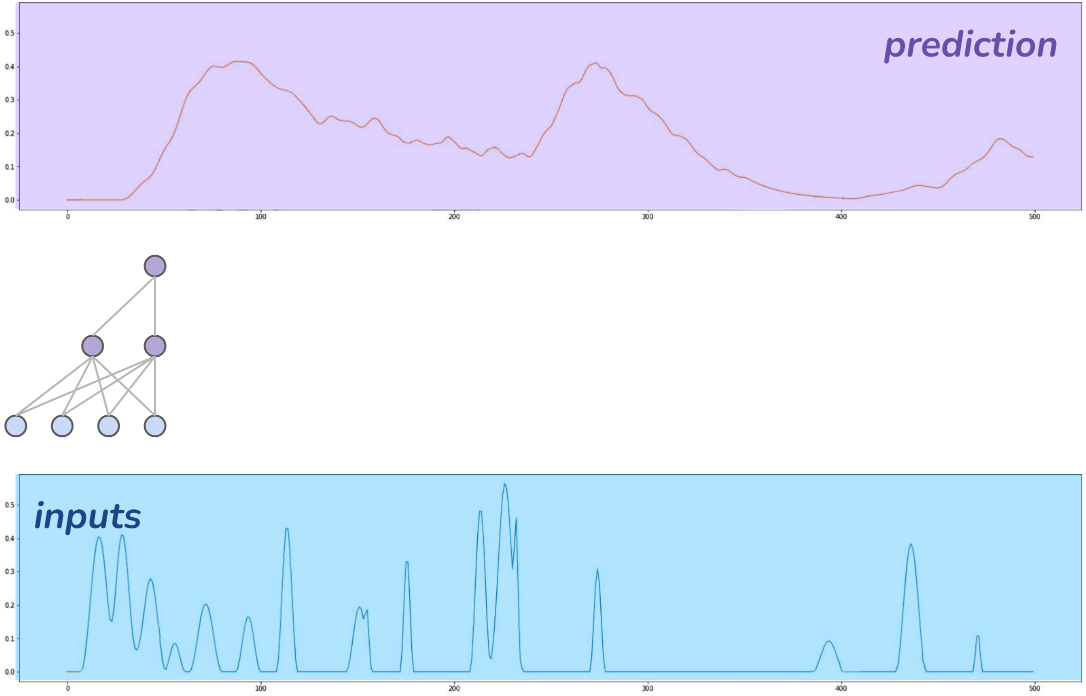
Simple feed-forward network



Sliding feed-forward network



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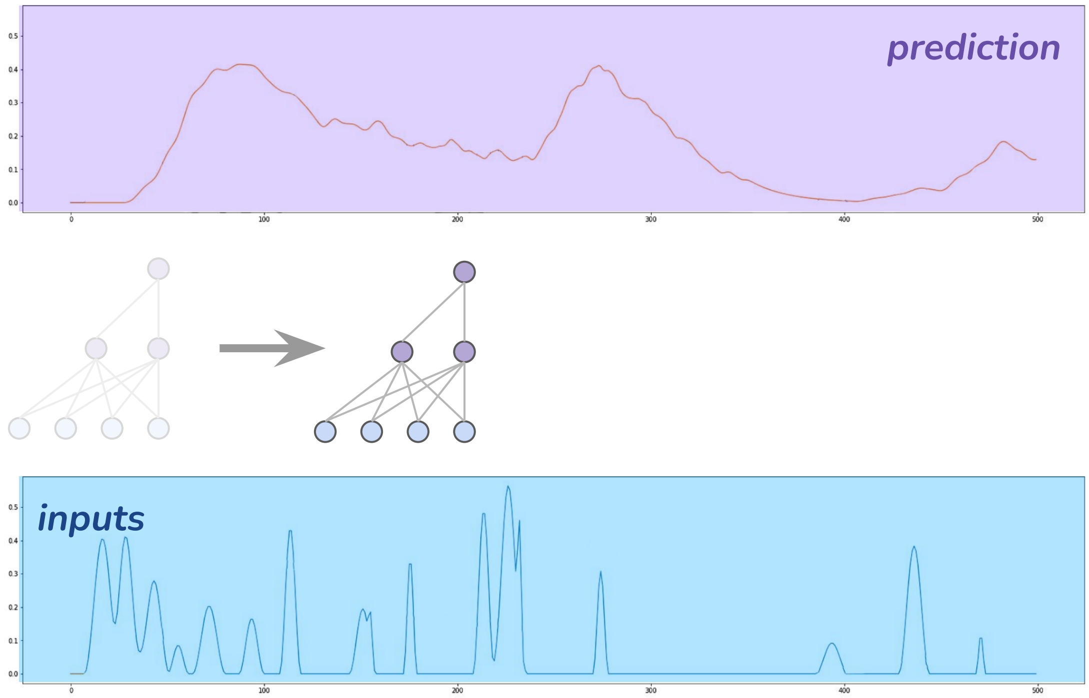

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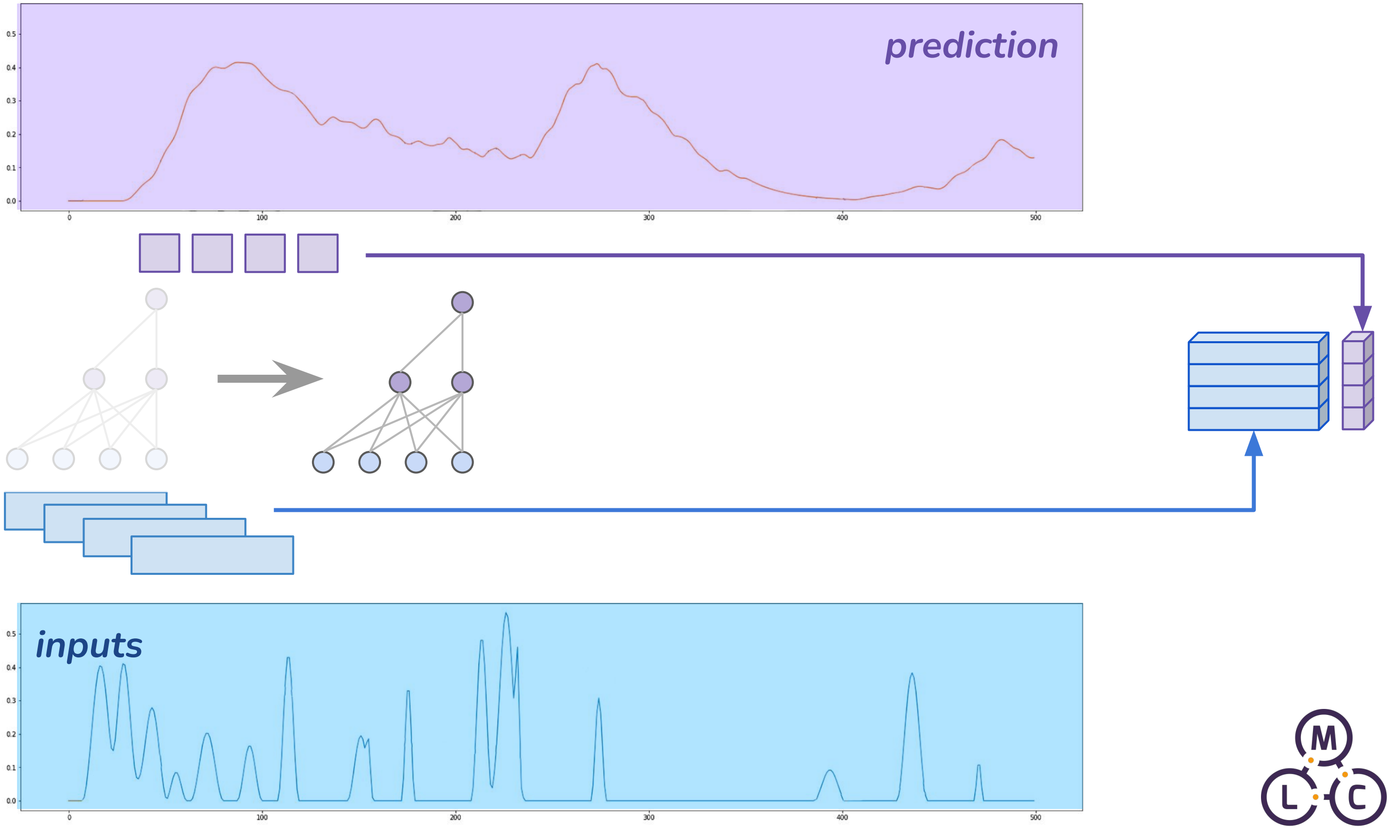

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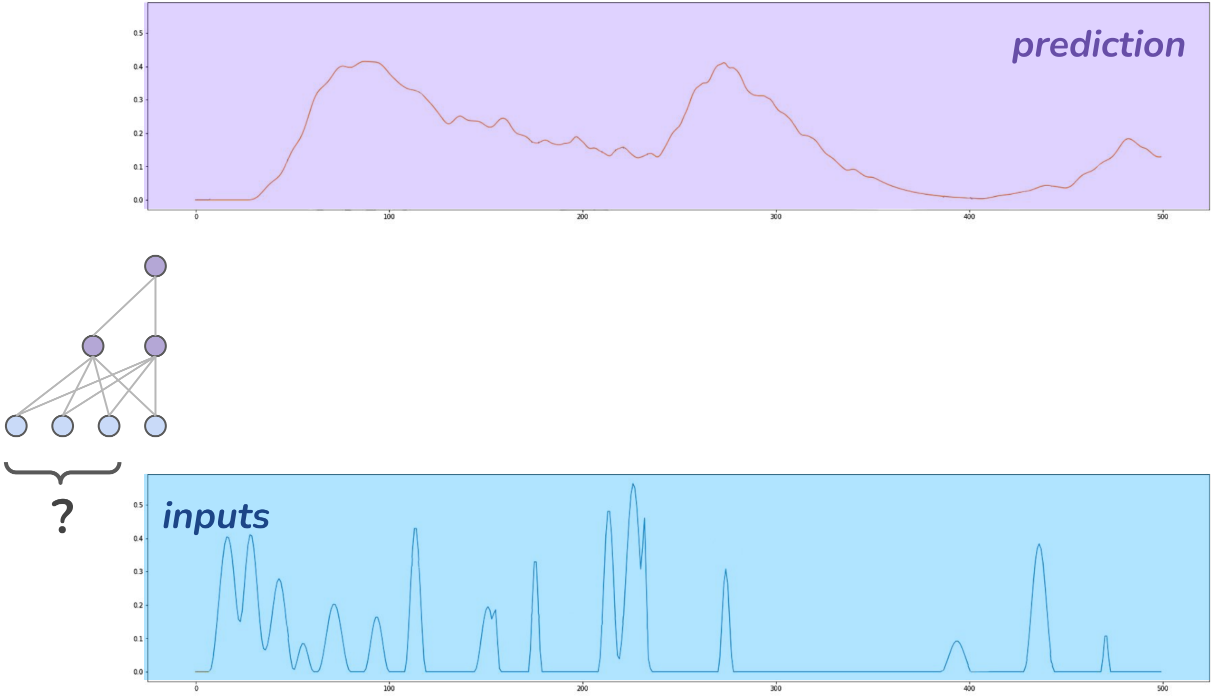

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Sliding feed-forward network

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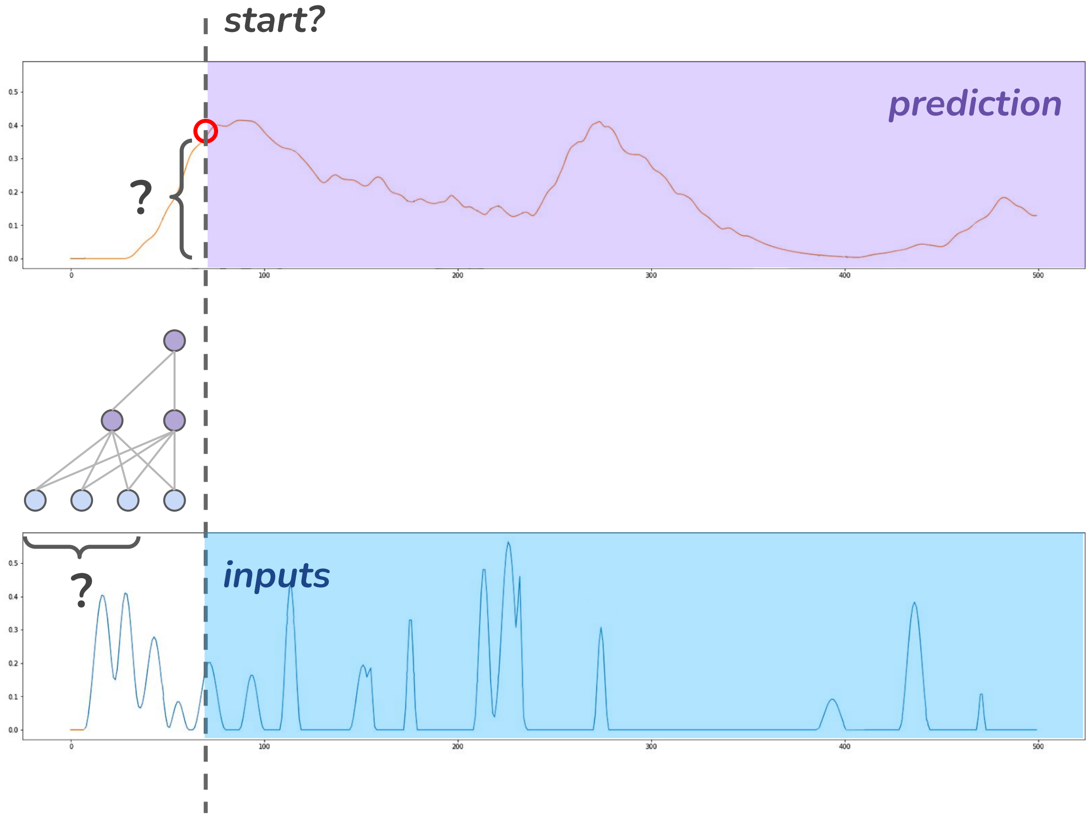
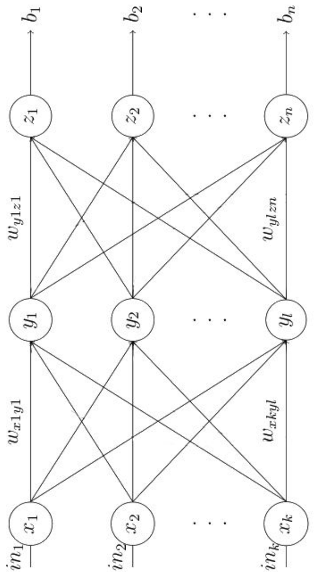
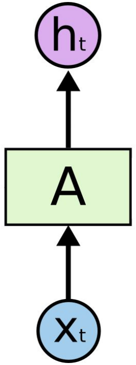
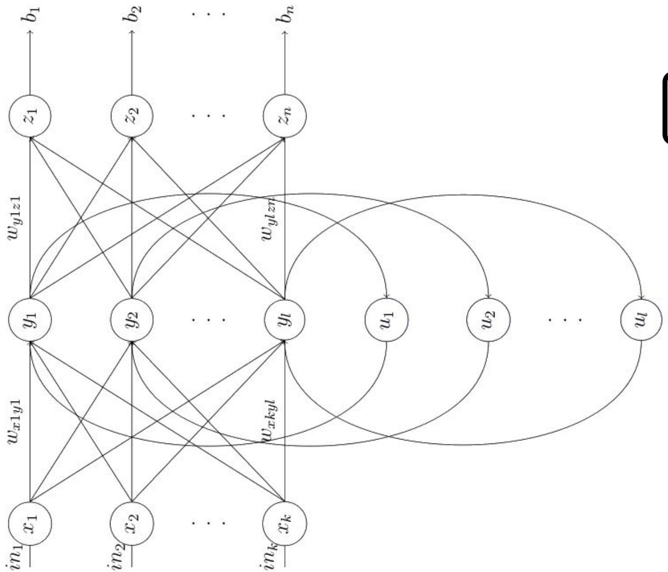
Sliding feed-forward network

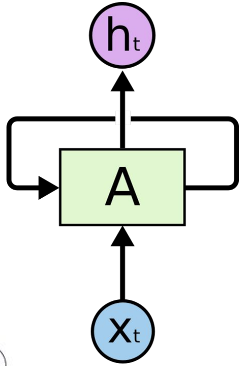


Recurrent Neural Networks



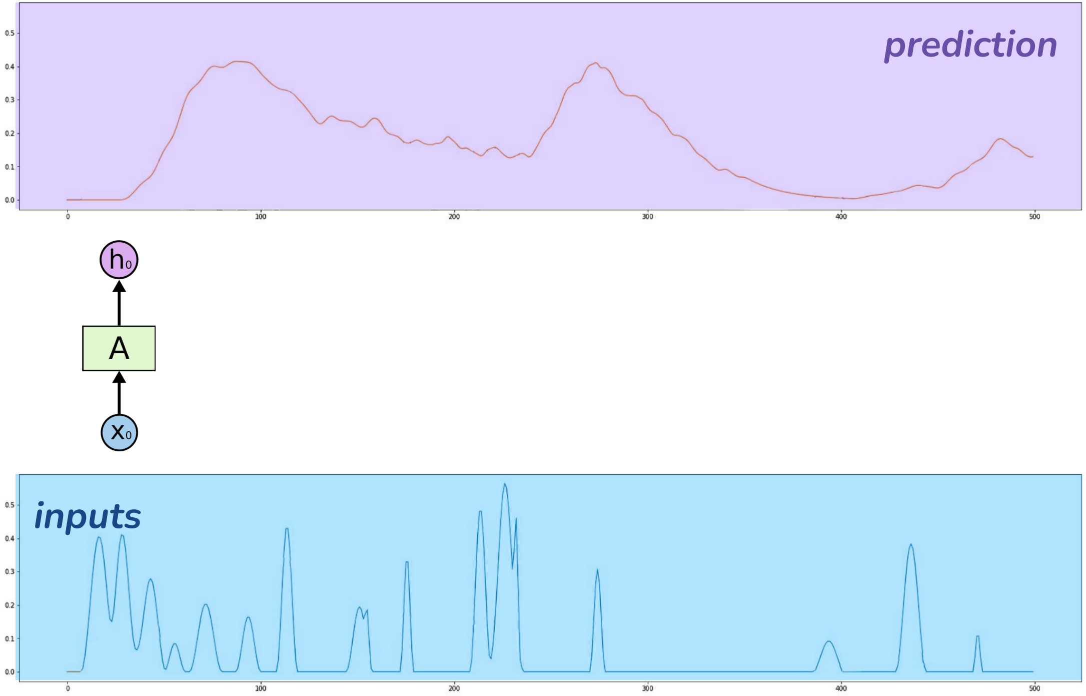






*http://colah.github.io/posts/2015-08-Understanding-LSTMs/

RNN for time series prediction



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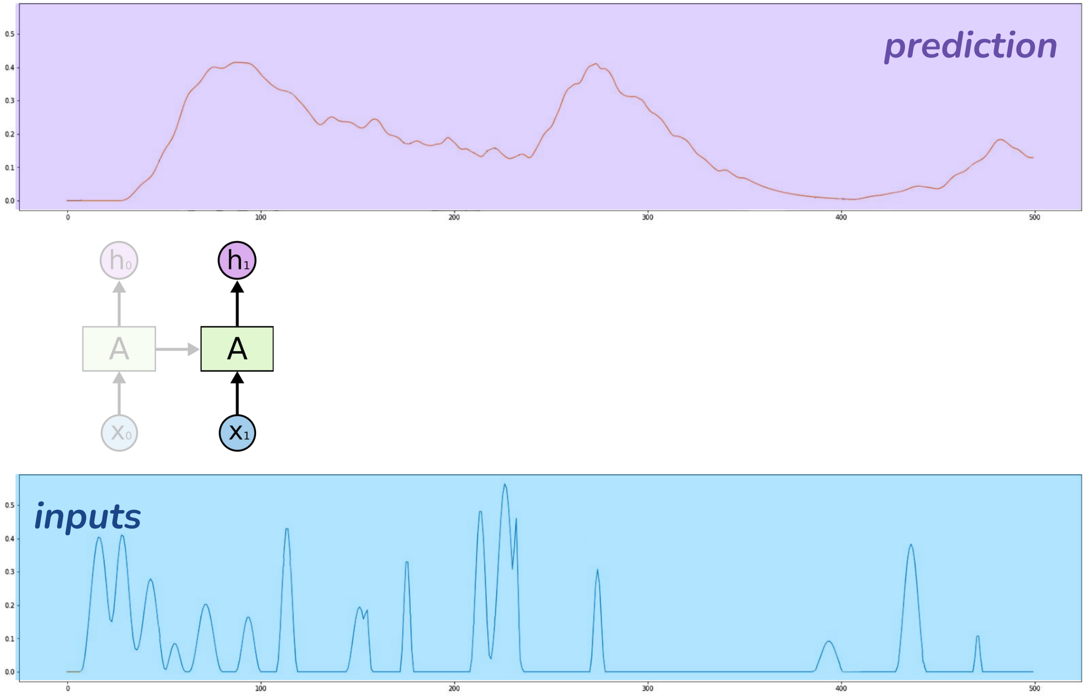
RNN for time series prediction



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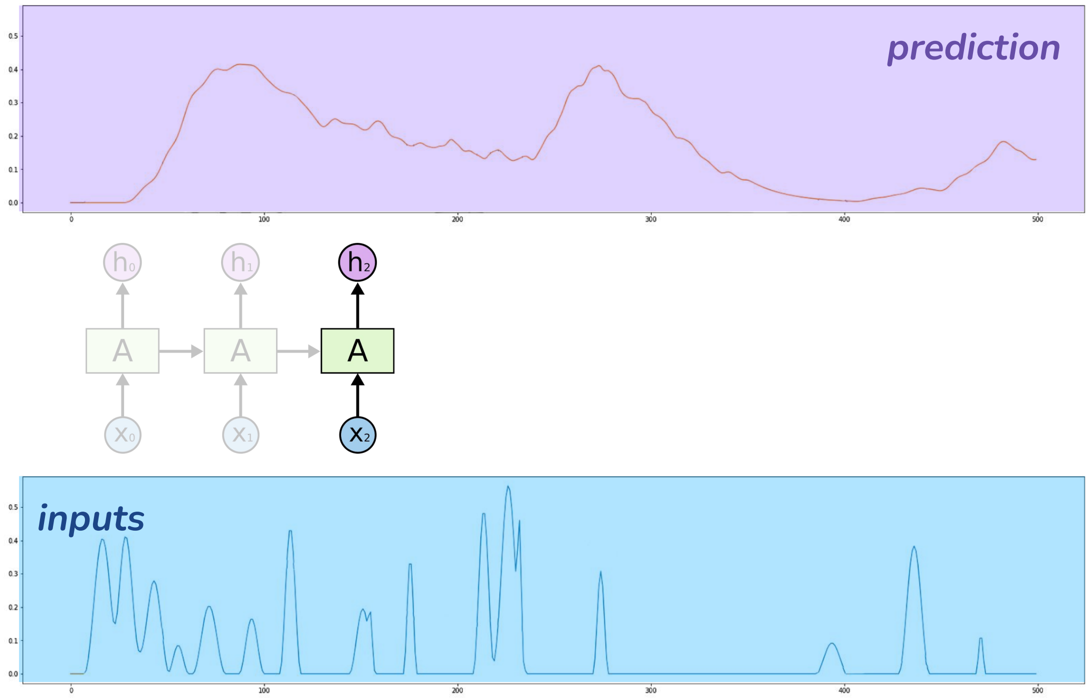
RNN for time series prediction



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RNN for time series prediction

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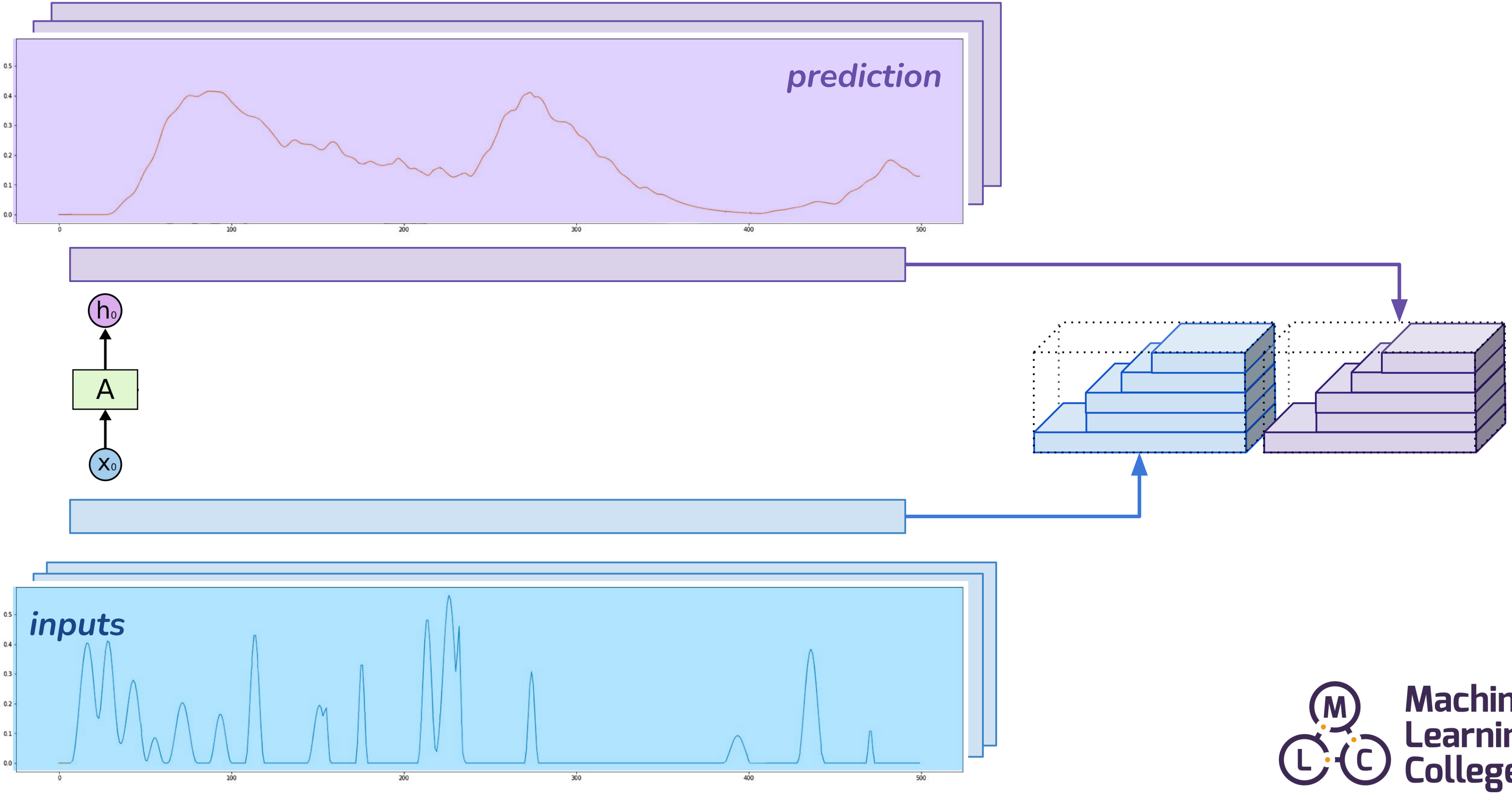
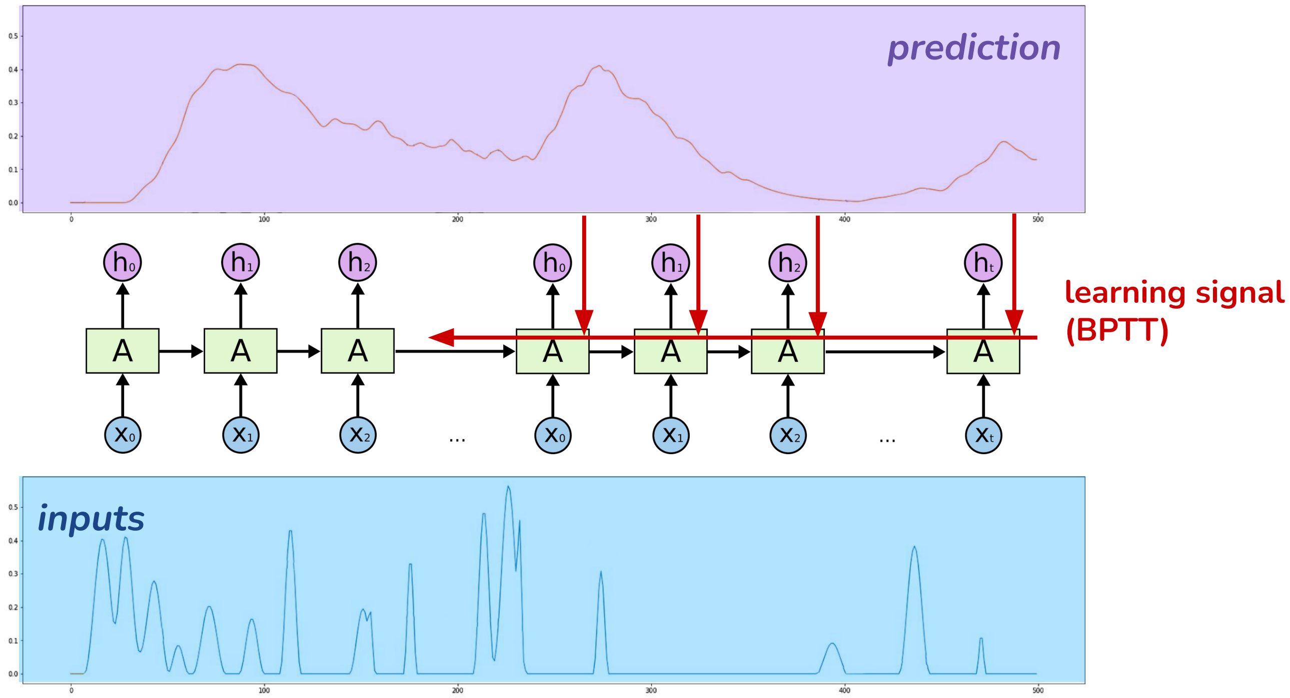
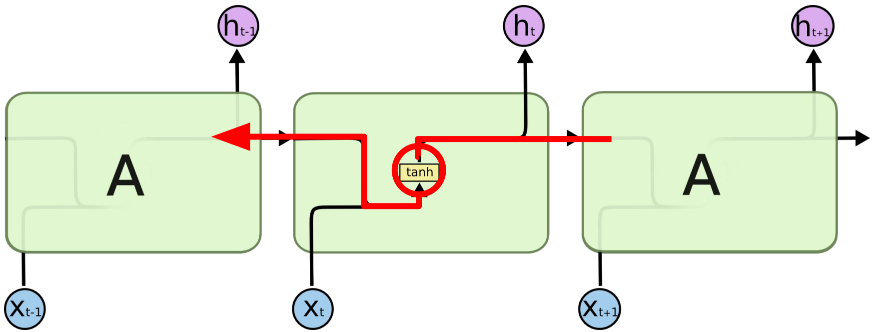
RNN for time series prediction

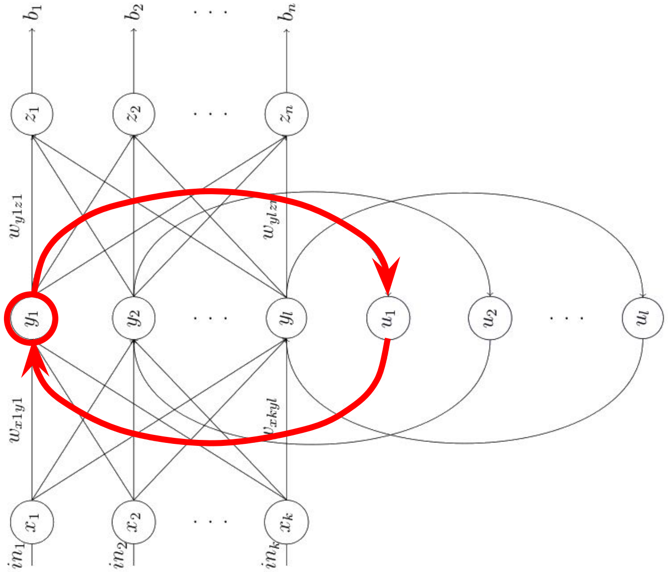


RNN for time series prediction



RNN – Vanishing gradients





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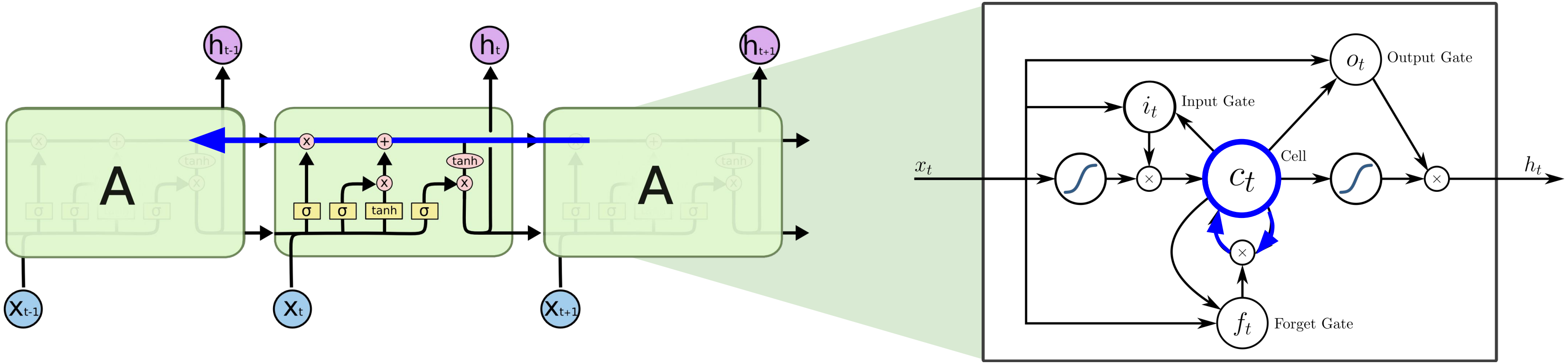
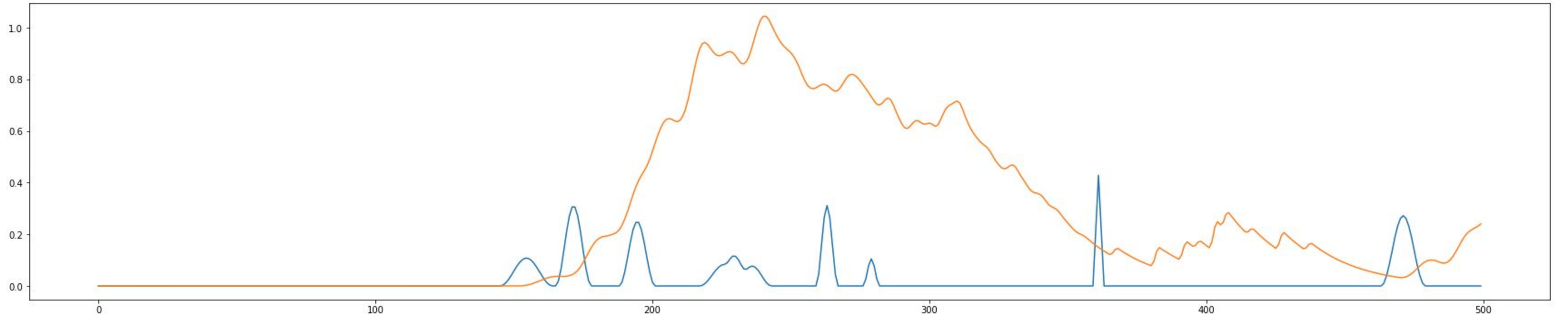
Long short-term memory – LSTM



*http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Rainfall-runoff example

rainfall_runoff.ipynb



- Test out neural networks on simple **generated rainfall-runoff dataset**
  - Simulated **long-time dependencies** in data
  - Test various neural network architectures
    - Flat feed-forward network
    - LSTM

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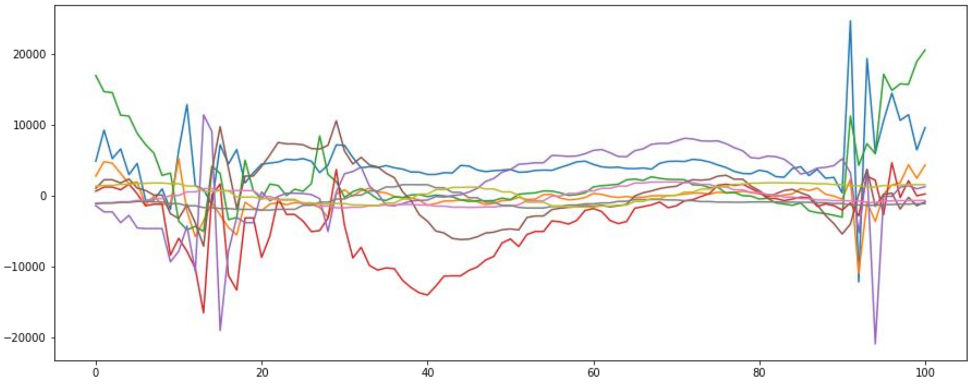
Trampoline jumping example

- Data preparation
  - Dataset normalization
  - Sequence padding
- Binary classification task
  - Target values & dimensions
  - Loss functions
- Training & evaluation
  - Inference visualization
  - Evaluation metrics



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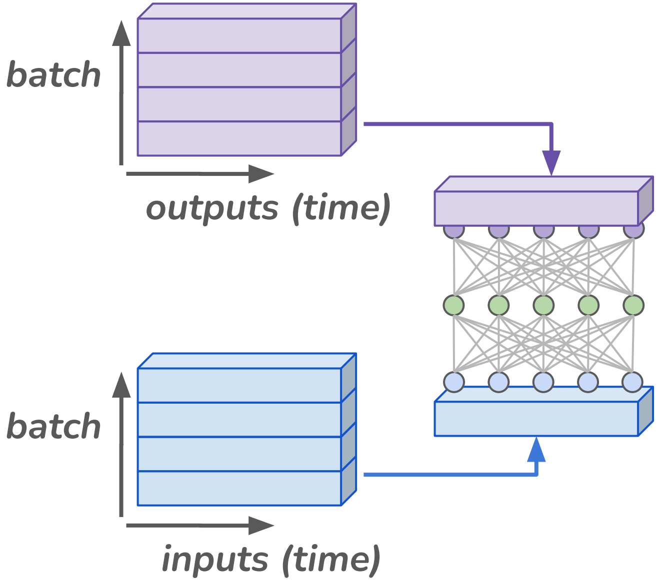
Tensors & dimentions – univariate regression

Flat NN = 2D training data



(B, T)⟶(B, T)

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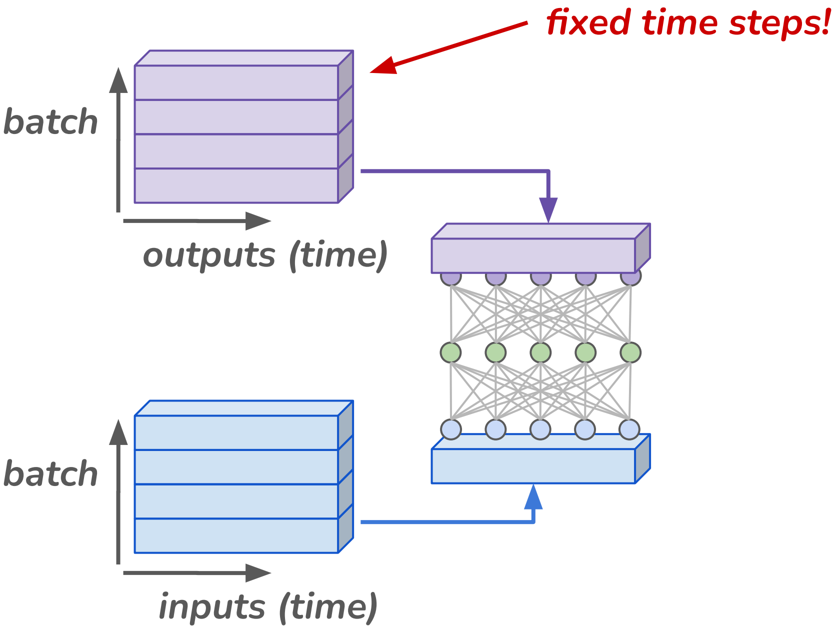
Tensors & dimentions – univariate regression

Flat NN = 2D training data



(B, T)⟶(B, T)

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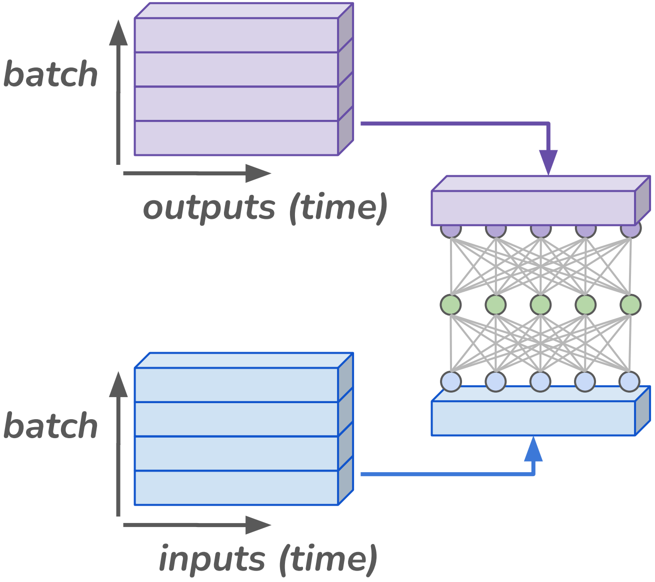
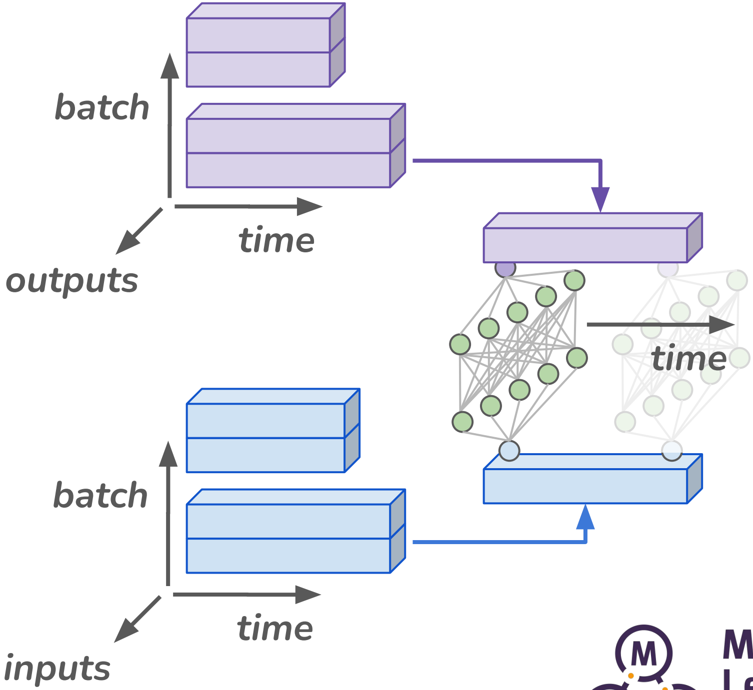
Tensors & dimentions – univariate regression

Flat NN = 2D training data



$(B, T) \longrightarrow (B, T)$

Recurrent NN = 3D training data



$(B, T, 1) \longrightarrow (B, T, 1)$

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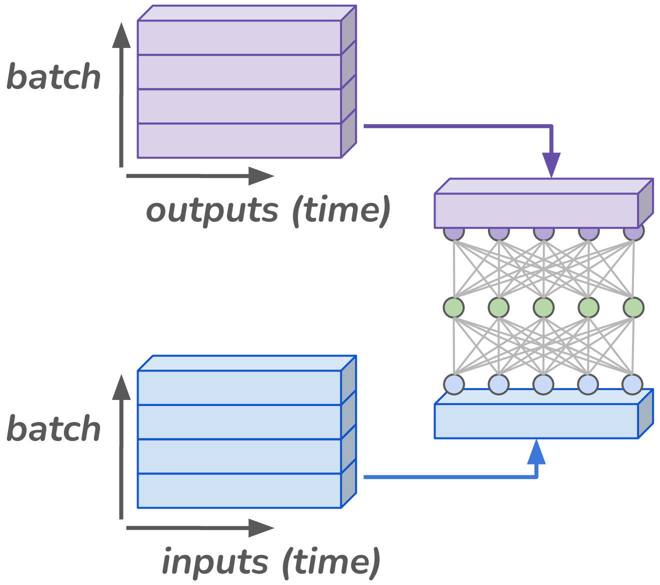
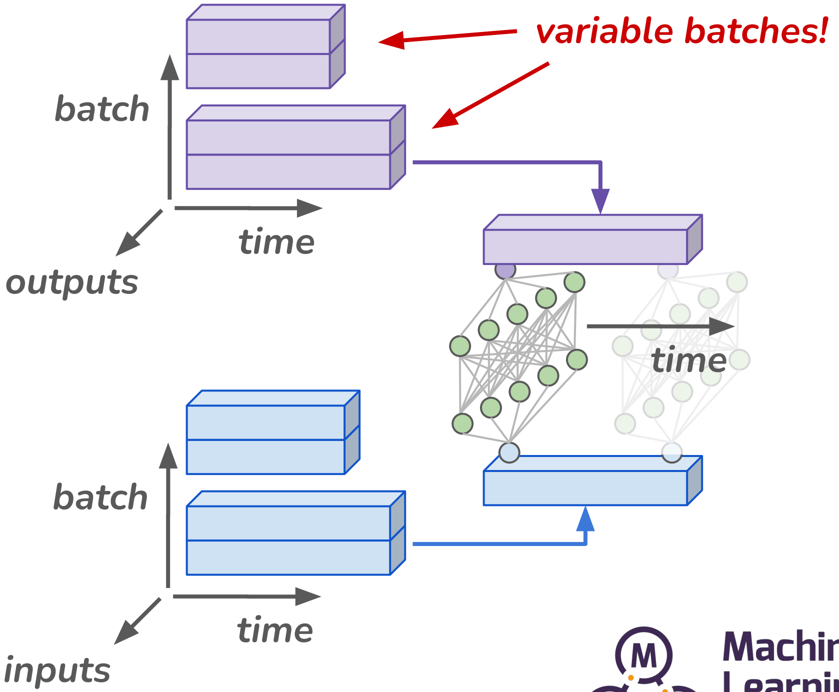
Tensors & dimentions – univariate regression

Flat NN = 2D training data



(B, T) ⟶ (B, T)

Recurrent NN = 3D training data



(B, T, 1) ⟶ (B, T, 1)

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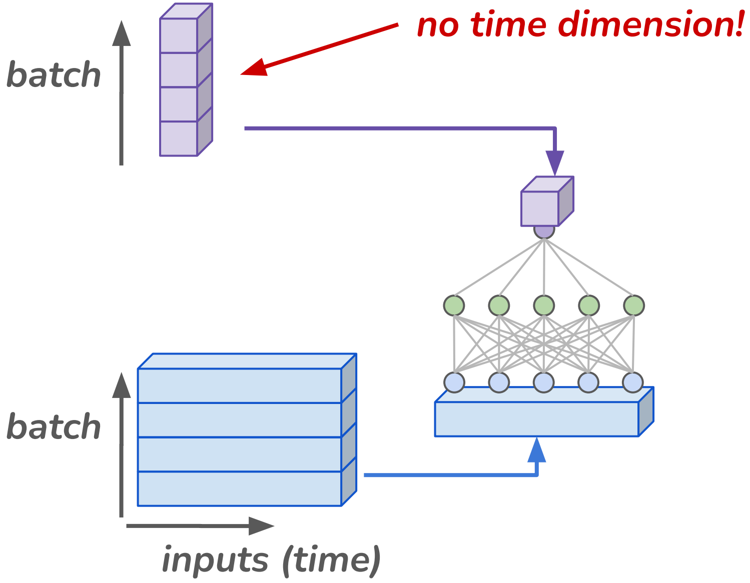
Tensors & dimentions – binary classification

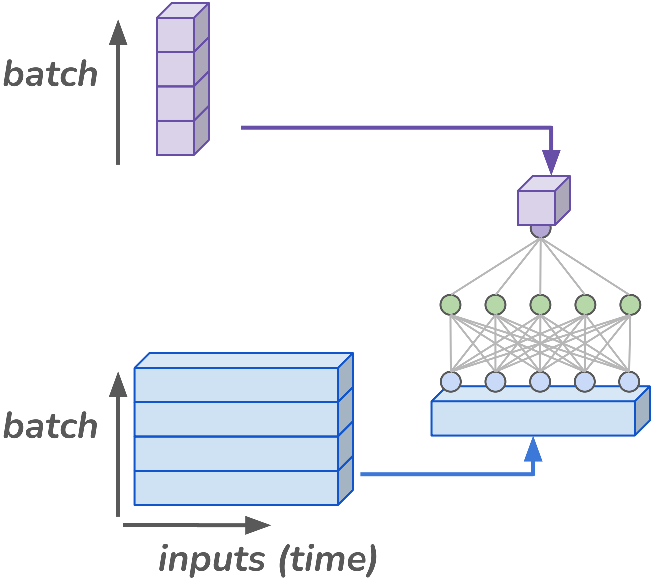
Flat NN = 2D training data



(B, T) ⟶ (B, 1)

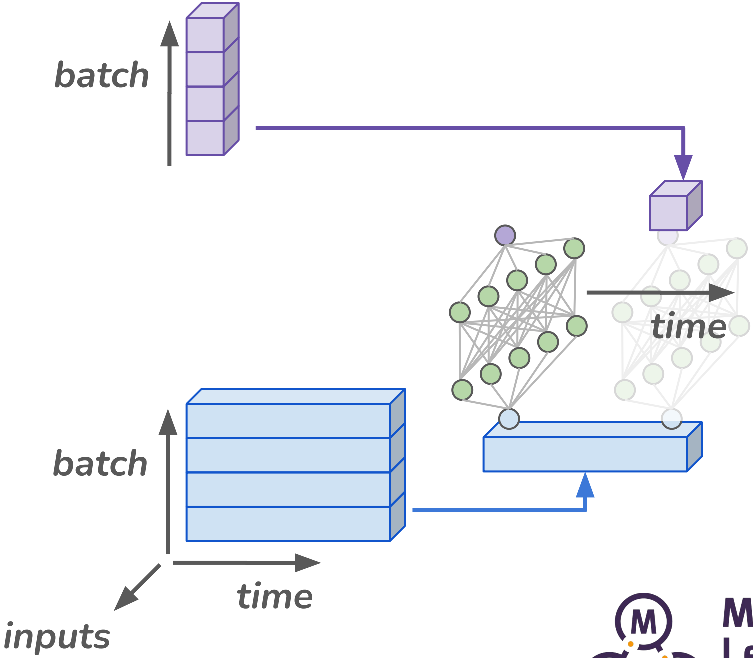
Tensors & dimentions – binary classification

Flat NN = 2D training data



(B, T) ⟶ (B, 1)

Recurrent NN = 3D training data



(B, T, 1) ⟶ (B, 1)

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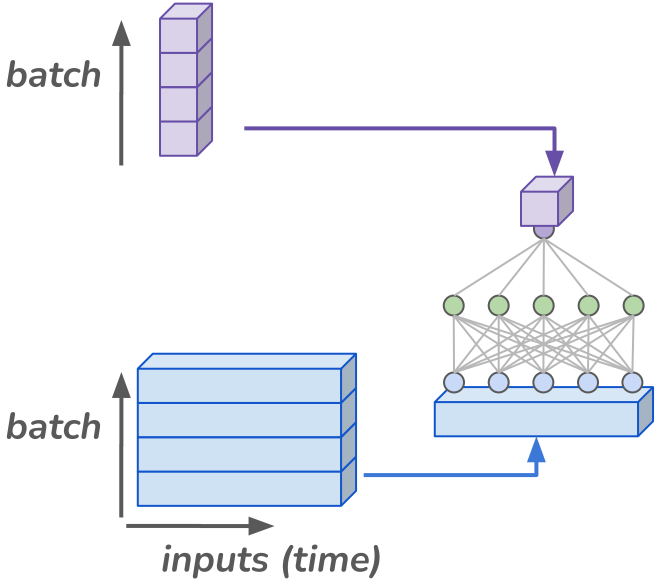
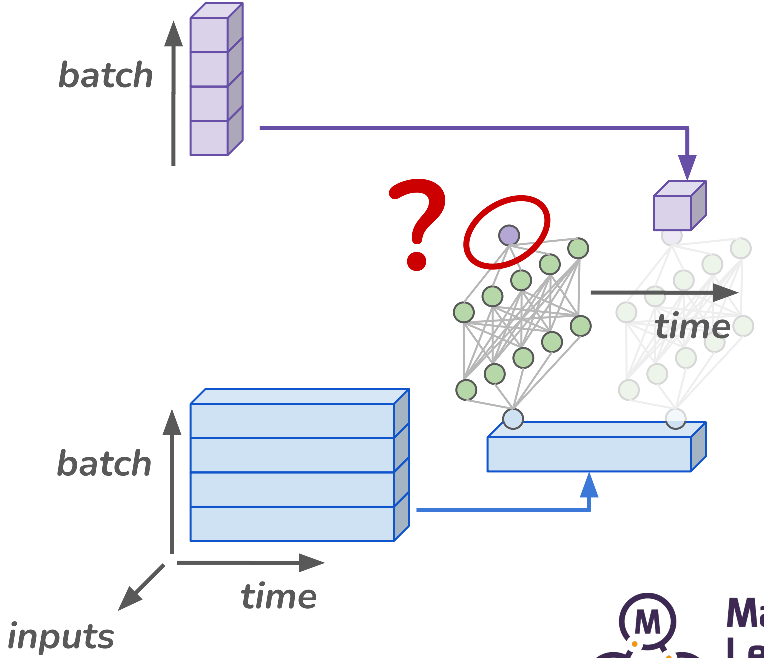
Tensors & dimentions – binary classification

Flat NN = 2D training data



(B, T)⟶(B, 1)

Recurrent NN = 3D training data



(B, T, 1)⟶(B, 1)

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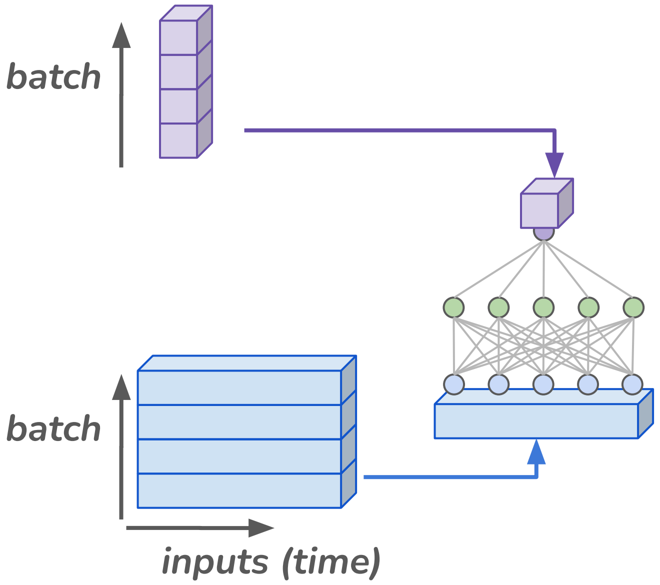
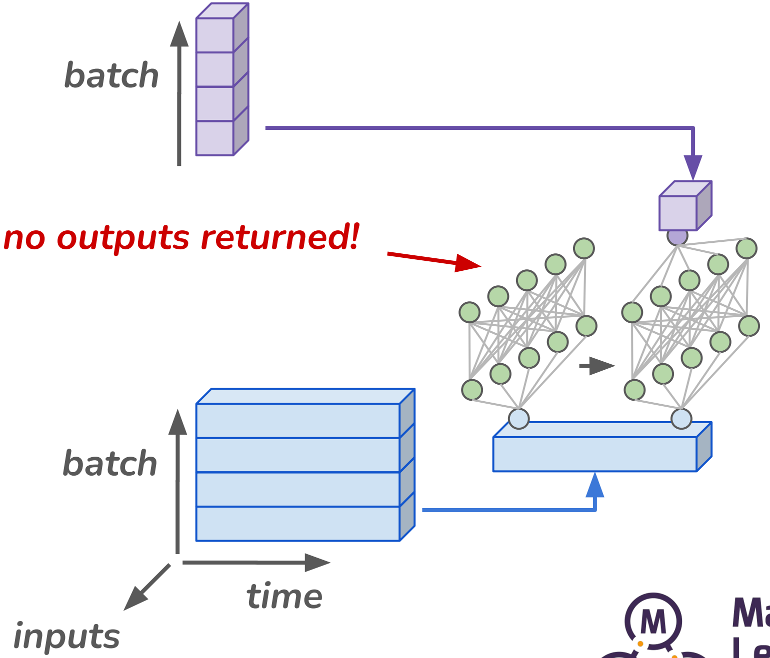
Tensors & dimentions – binary classification

Flat NN = 2D training data



(B, T)⟶(B, 1)

Recurrent NN = 3D training data



(B, T, 1)⟶(B, 1)

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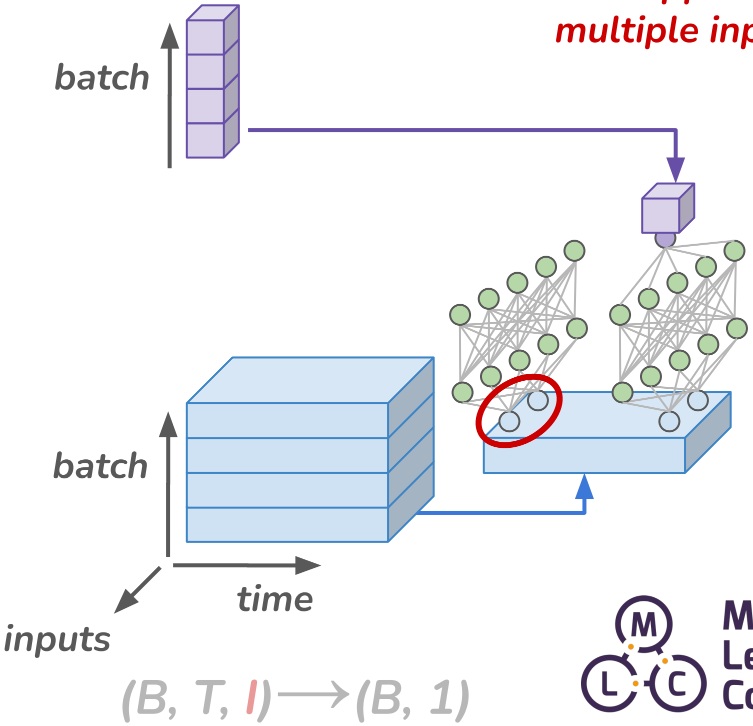
Tensors & dimentions – multivariate b. classification

Flat NN = 2D training data

?

Recurrent NN = 3D training data

natural support for multiple inputs



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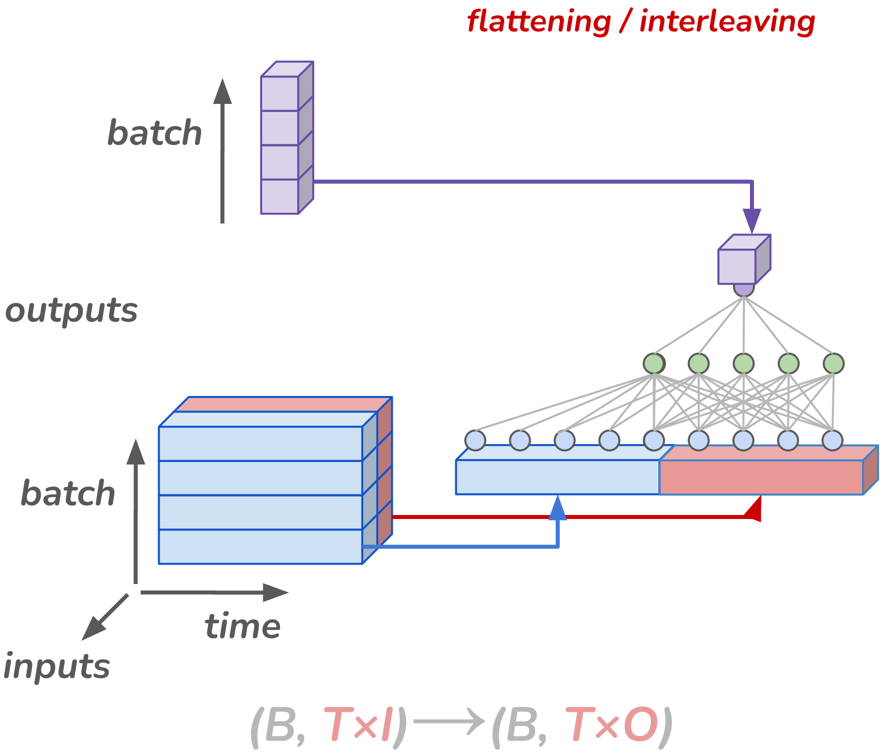
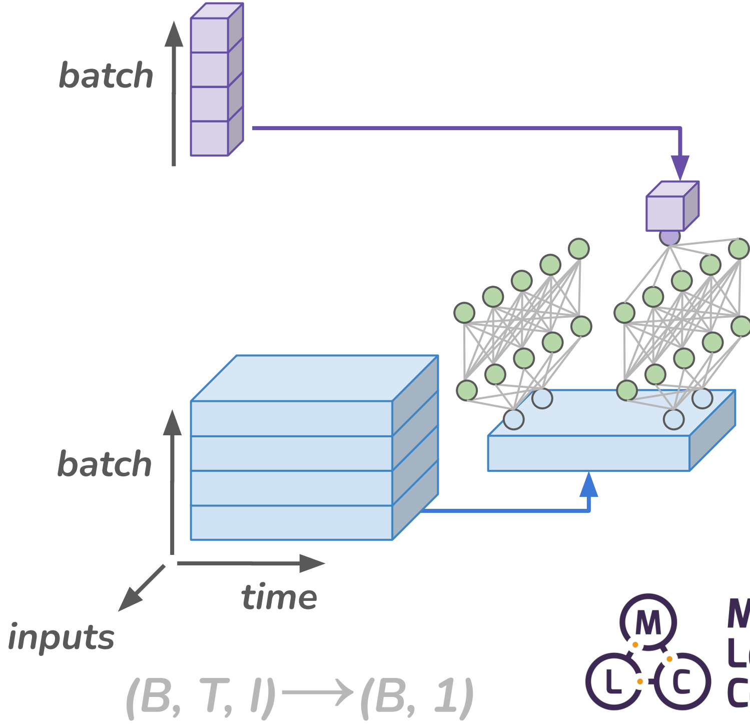
Tensors & dimentions – multivariate b. classification

Flat NN = 3D⟶2D training data



Recurrent NN = 3D training data



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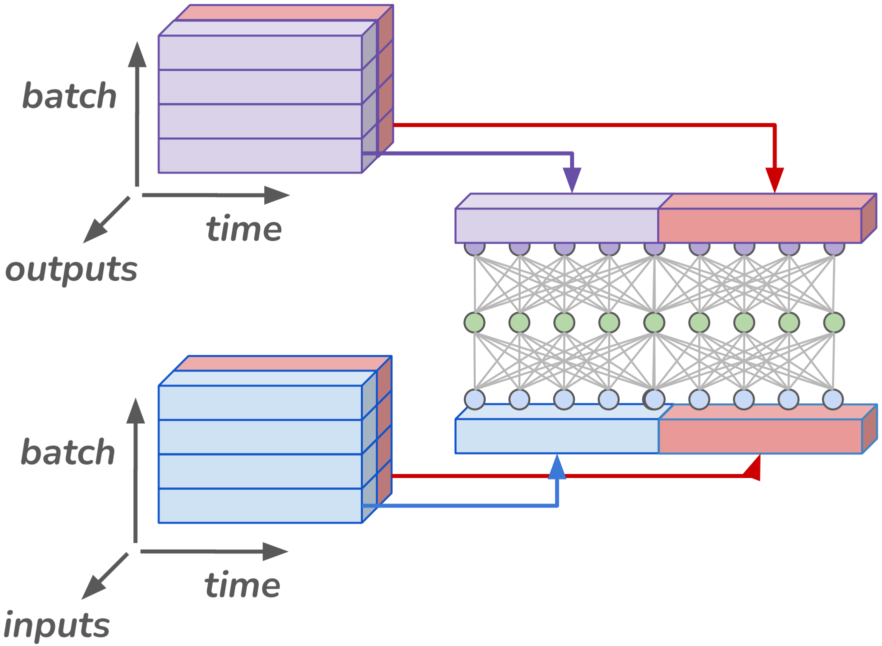
Tensors & dimentions – multivariate regression

Flat NN = 3D⟶2D training data

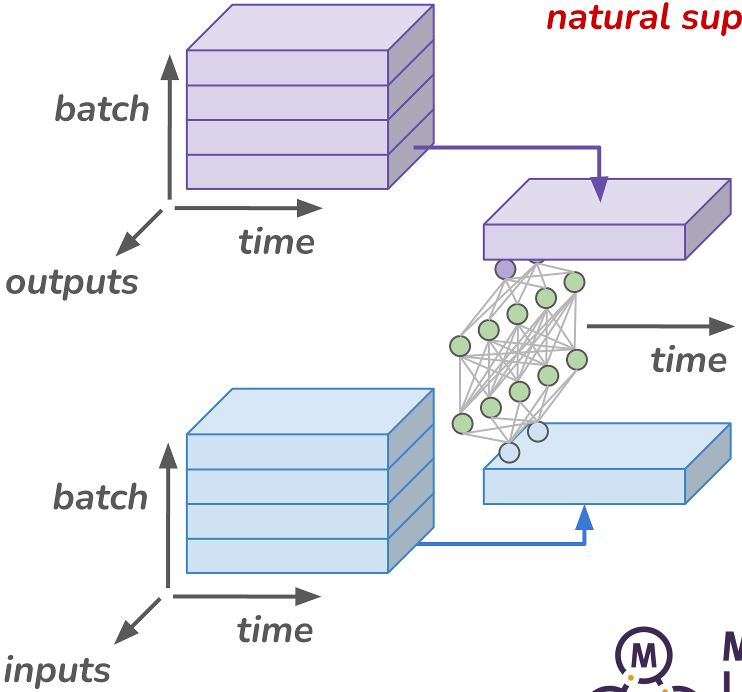
flattening / interleaving



$(B,\ T\times I) \longrightarrow (B,\ T\times O)$

Recurrent NN = 3D training data

natural support



$(B,\ T,\ I) \longrightarrow (B,\ T,\ O)$

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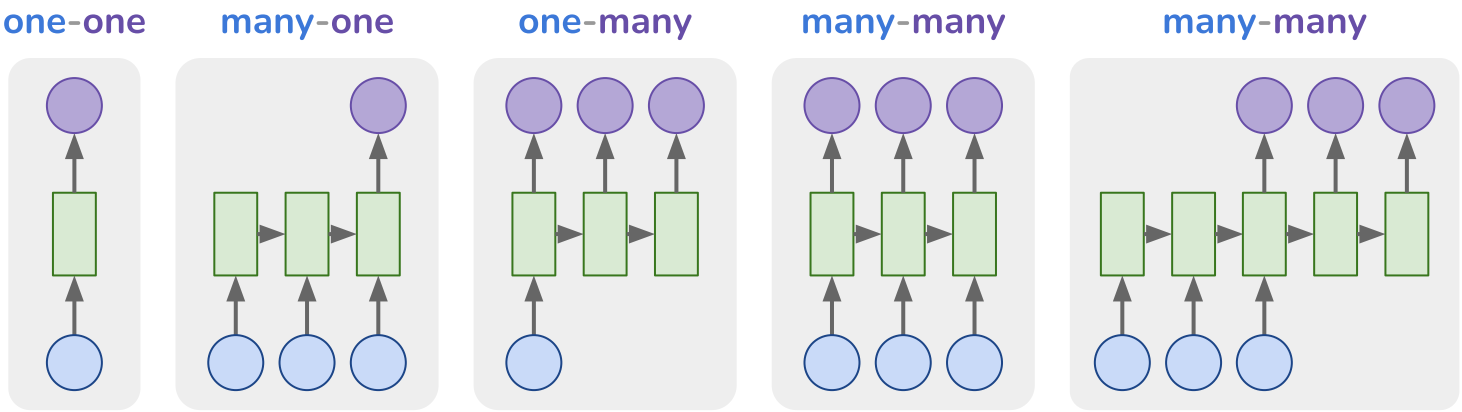
RNN and sequence data



sequence classification

image captioning

time series prediction

machine translation

*http://karpathy.github.io/2015/05/21/rnn-effectiveness/

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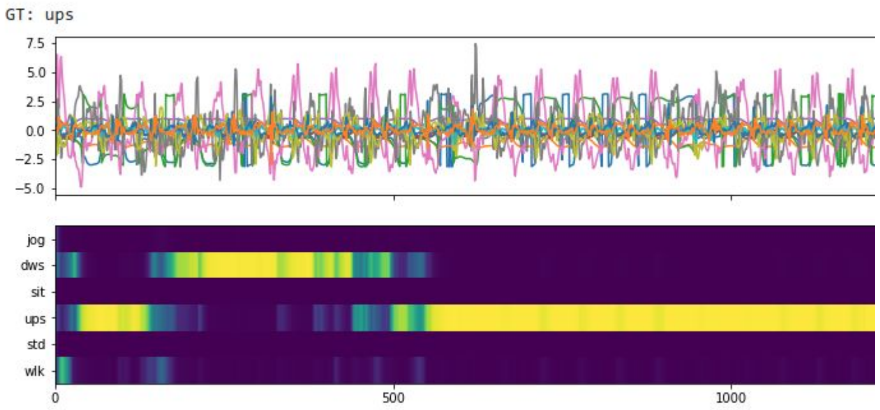
Motion sensing example

- Data preparation
  - Dataset normalization
  - Slicing long sequences
- Categorical classification task
  - Predict activity type
  - Use correct activation & loss function
- Training & evaluation
  - Try different architectures
  - Evaluate resuslt with standard metrics
- Secondary task
  - Subject identification



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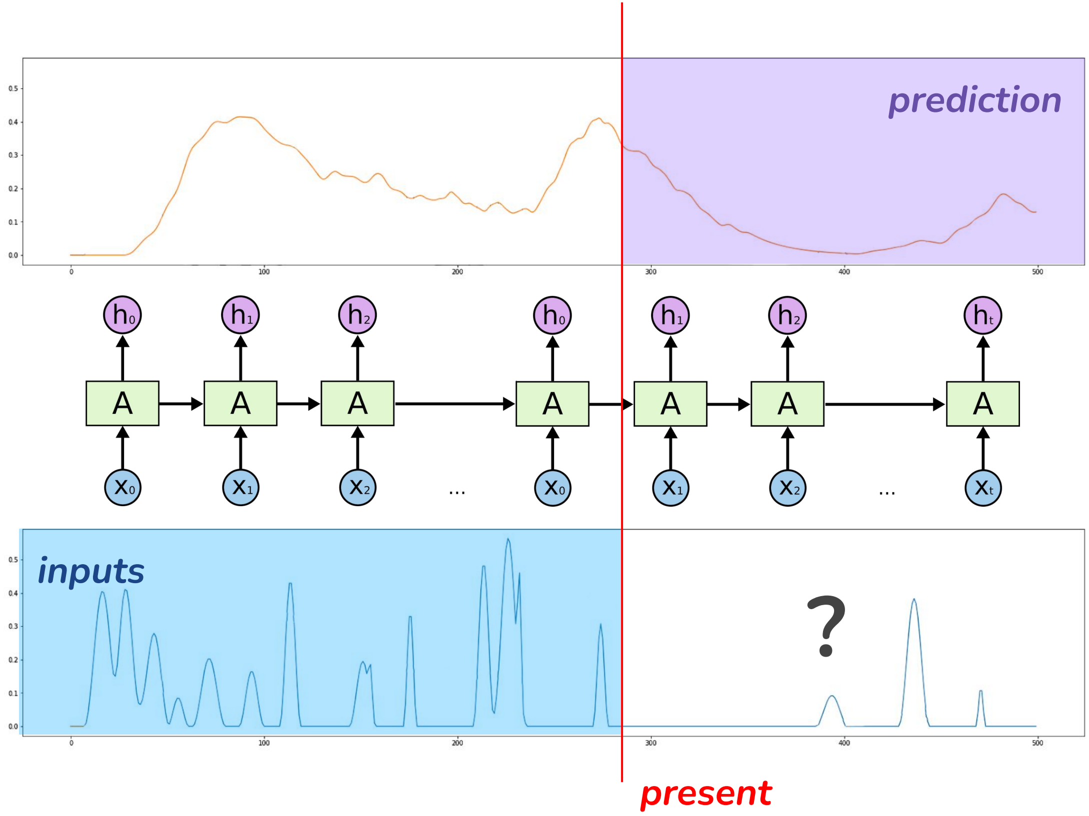
Forecasting



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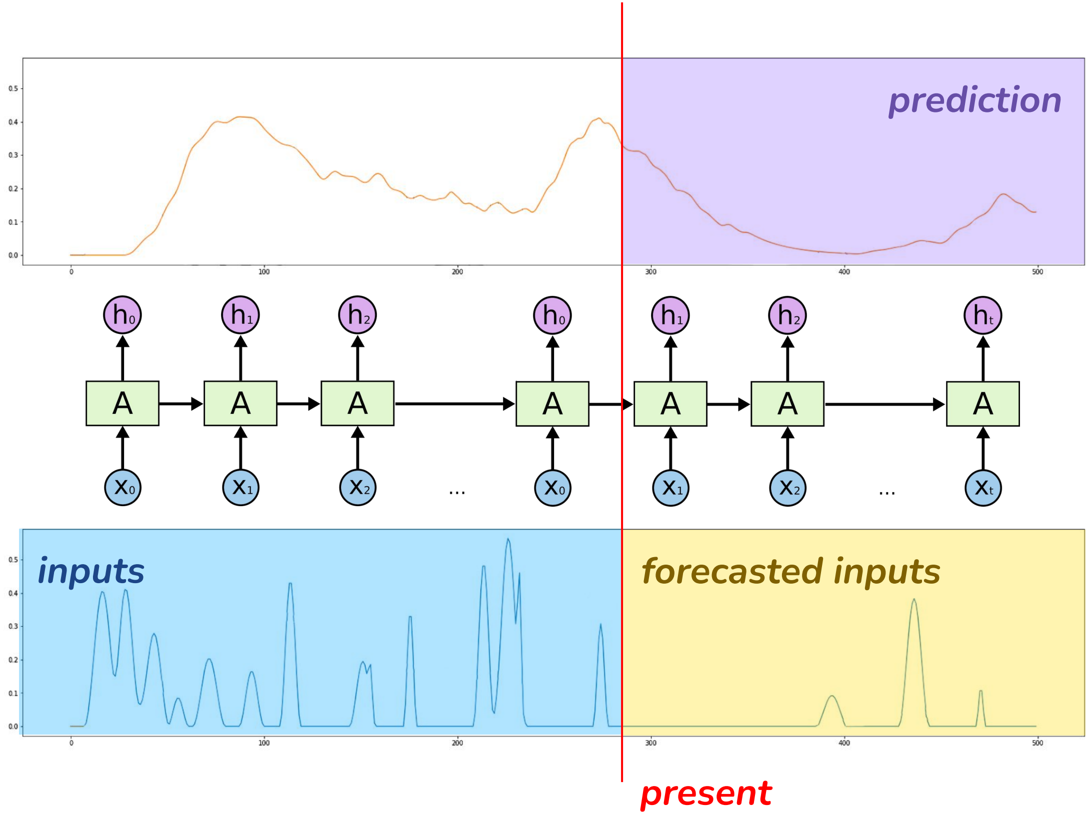
Forecasting



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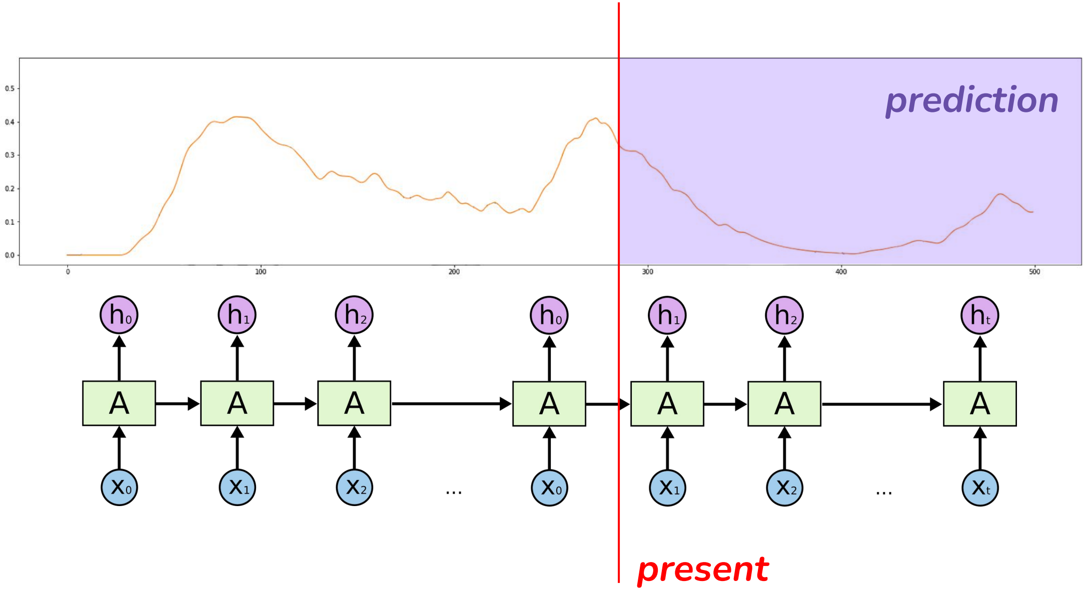
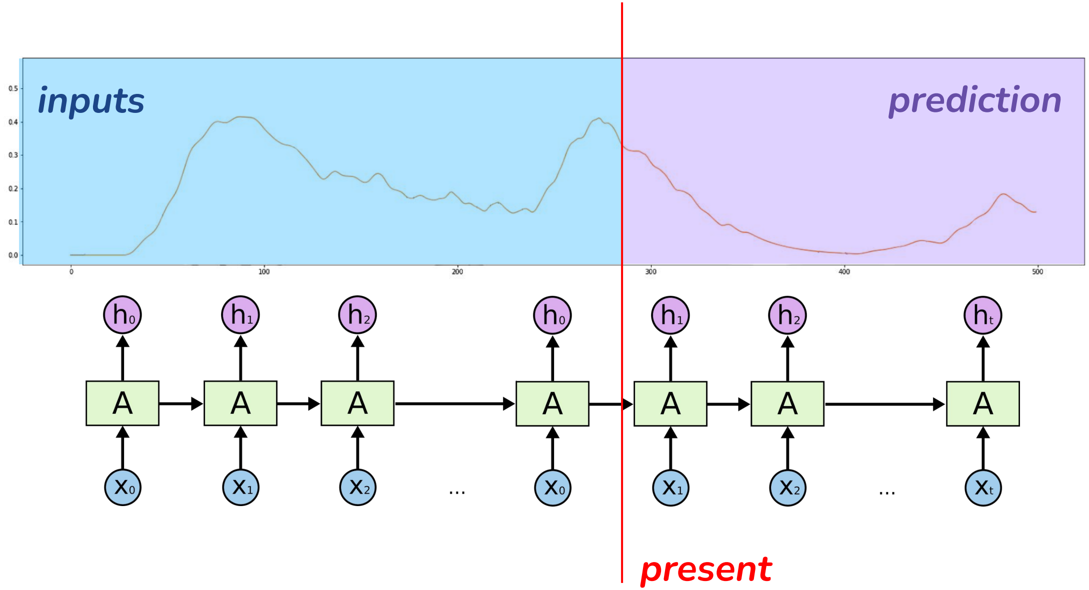
Forecasting



Forecasting



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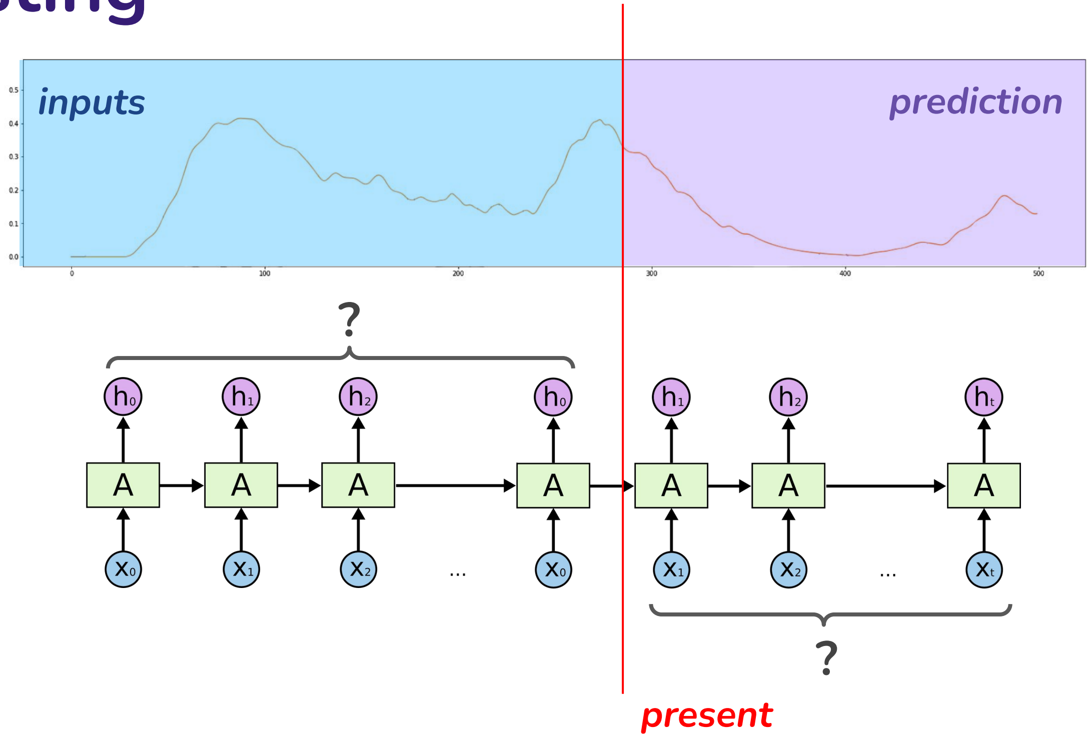
Forecasting



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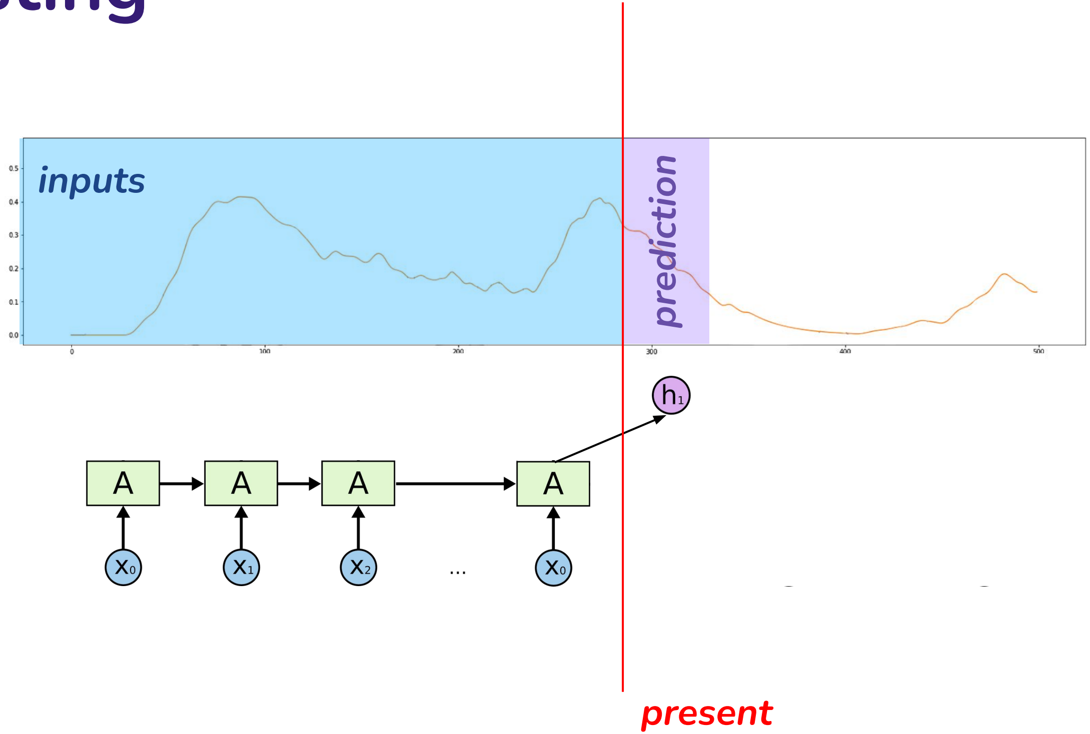
Forecasting



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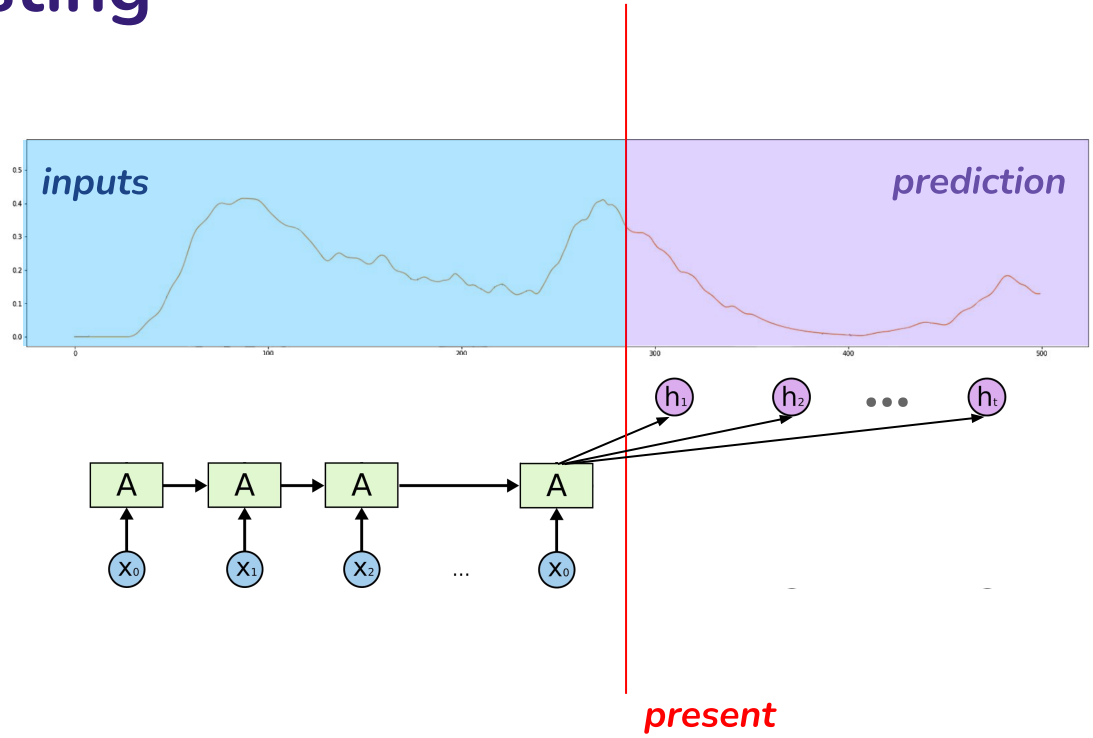
Forecasting



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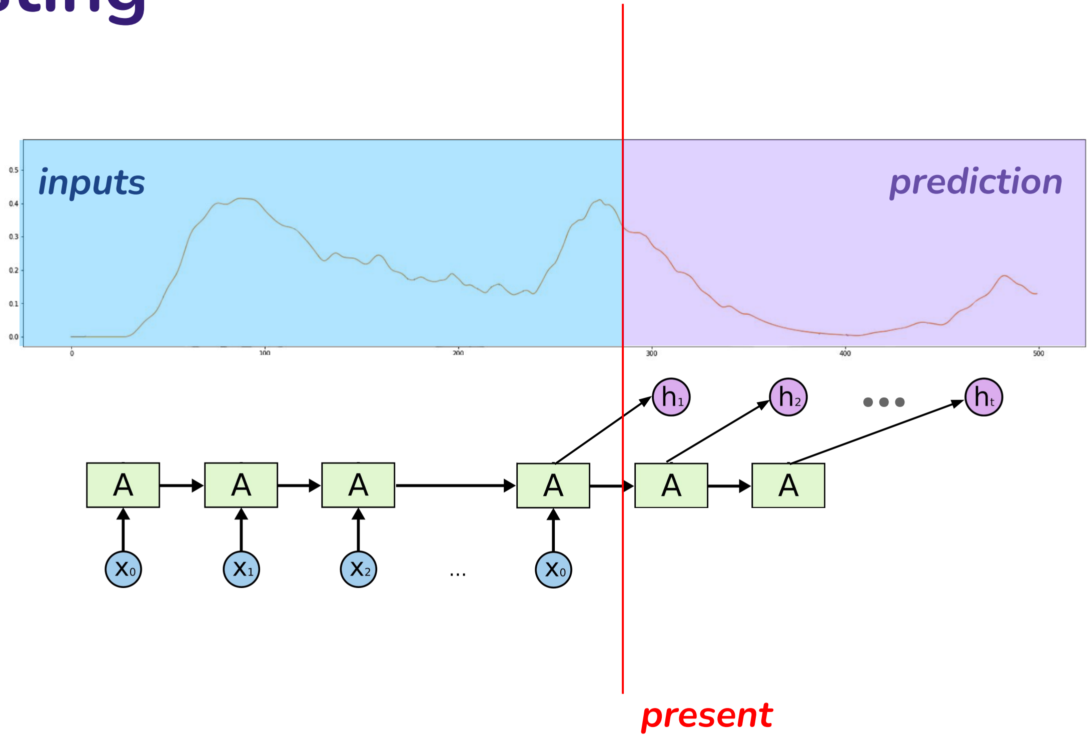
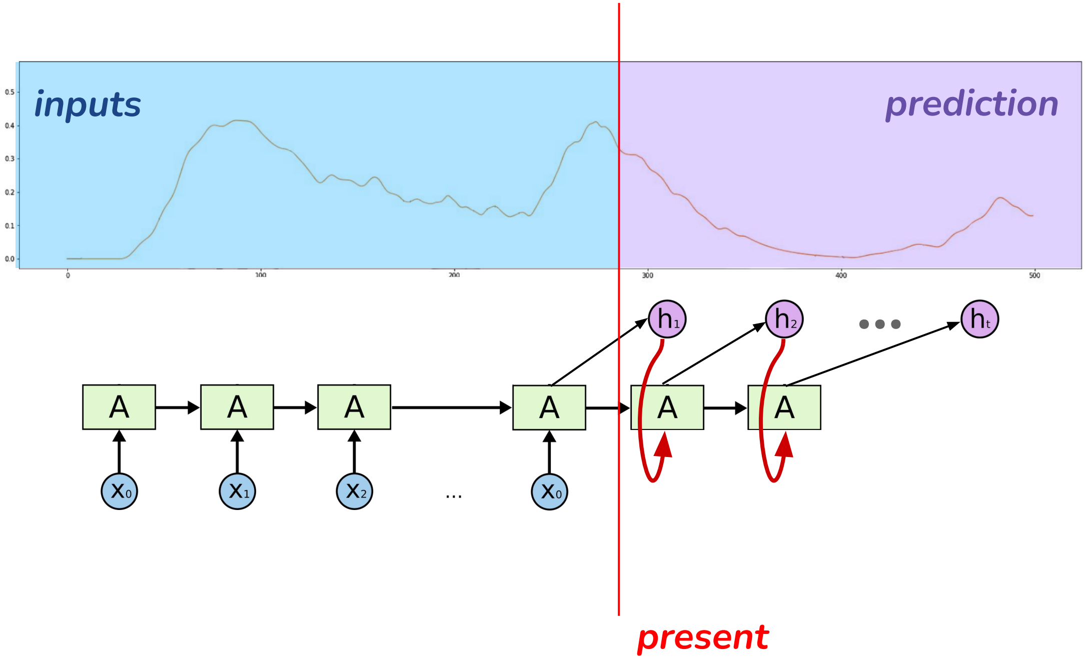
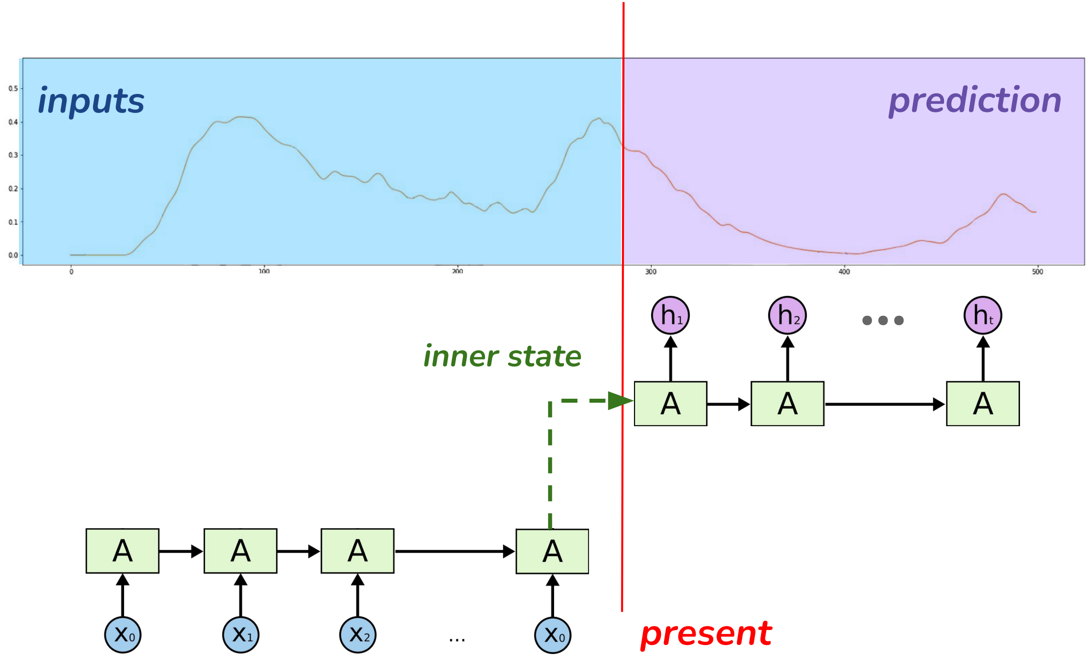
Forecasting



Forecasting



Forecasting – encoder & decoder



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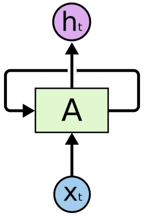
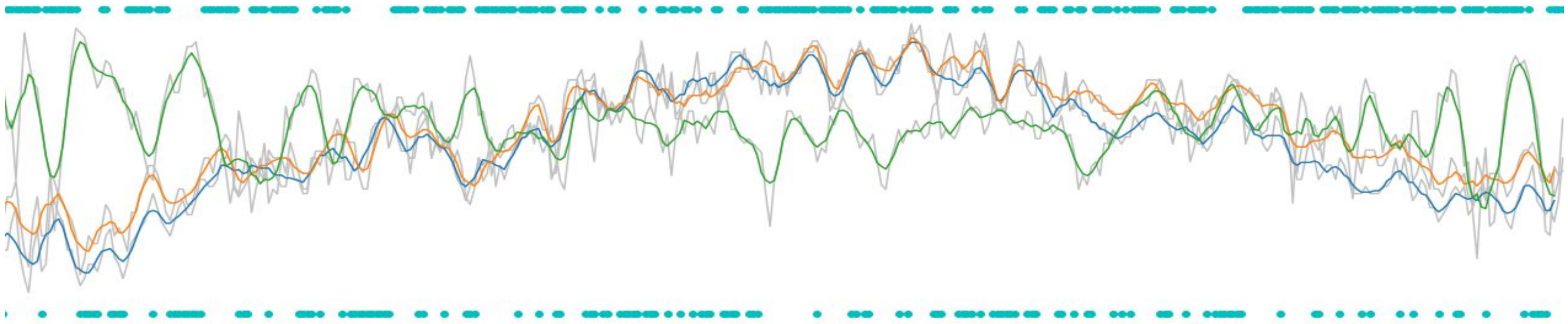
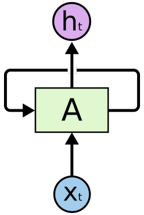
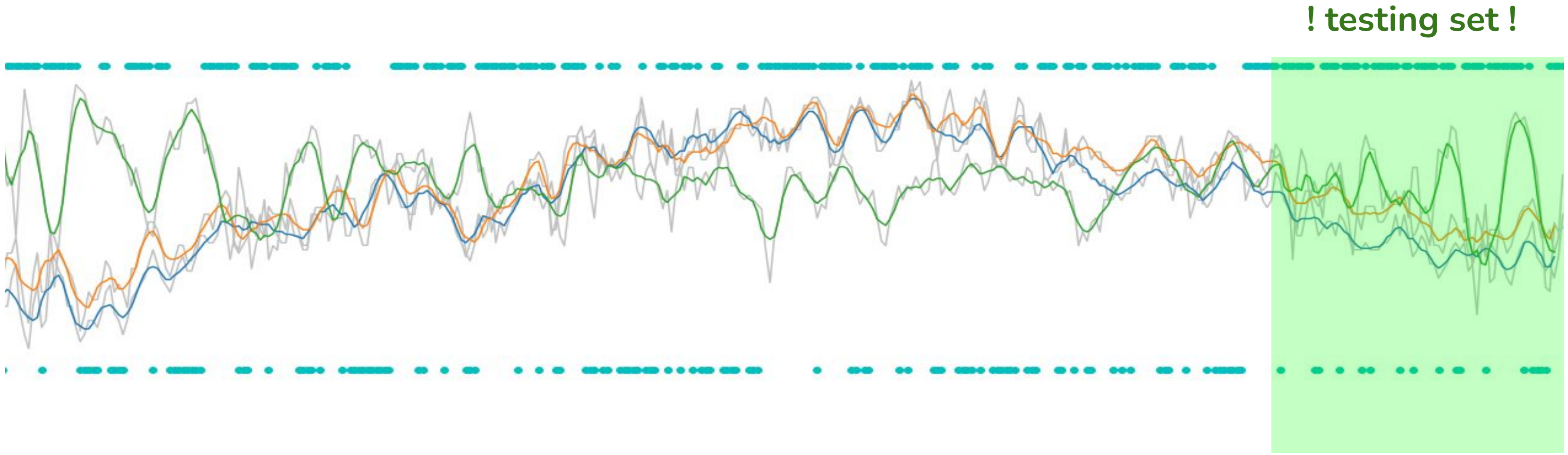
Training set construction



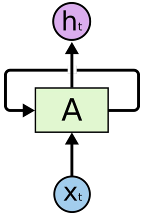


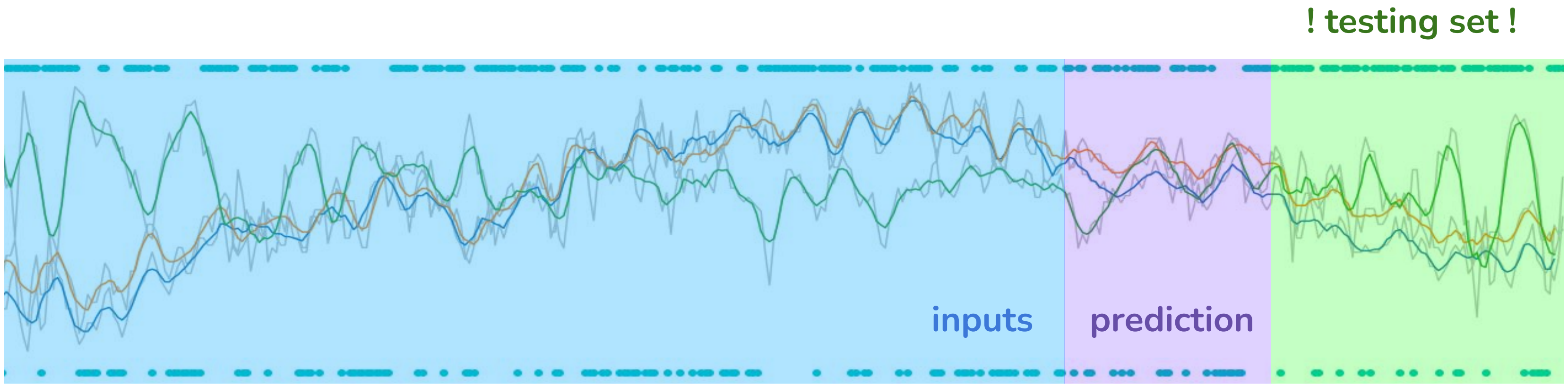
Training set construction



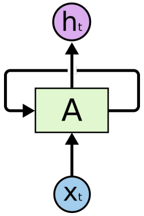


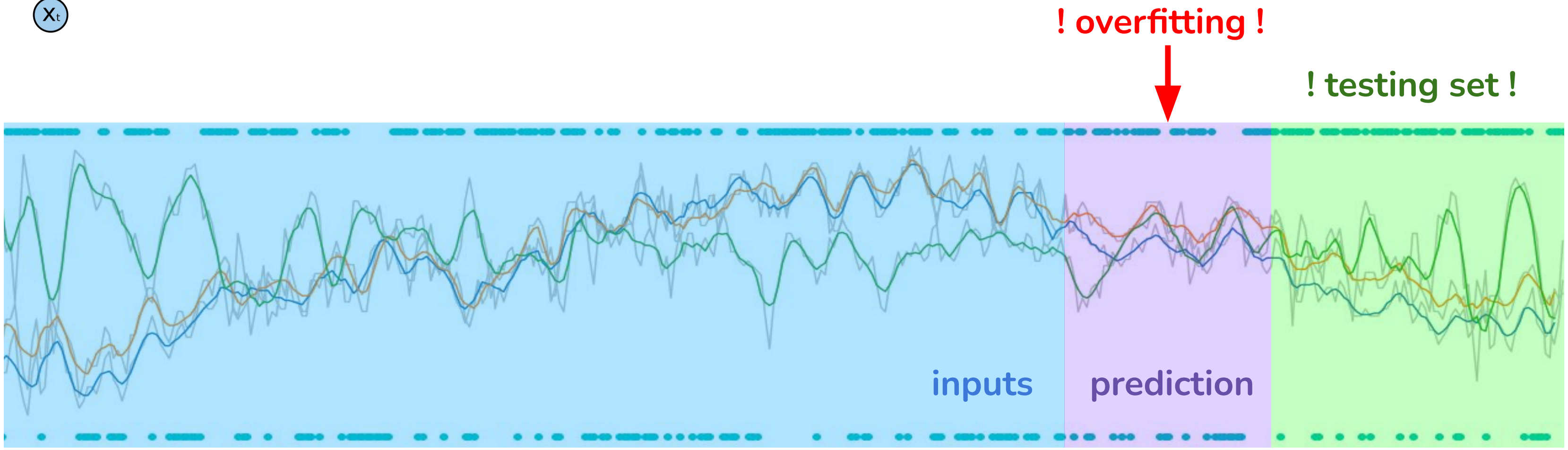
Training set construction



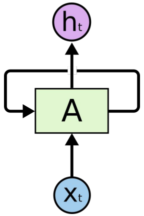


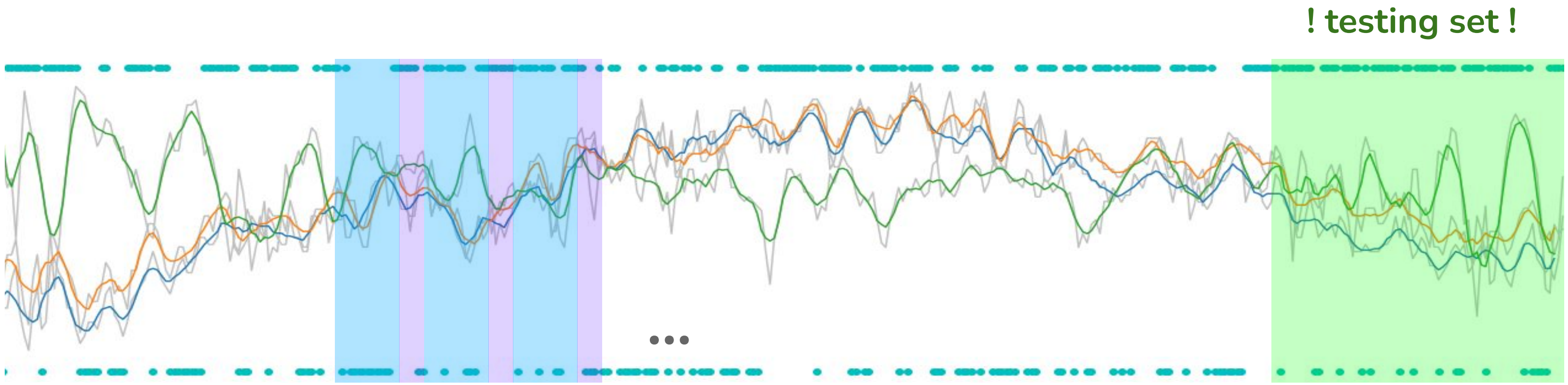
Training set construction



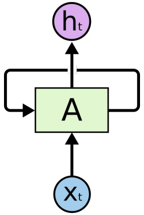


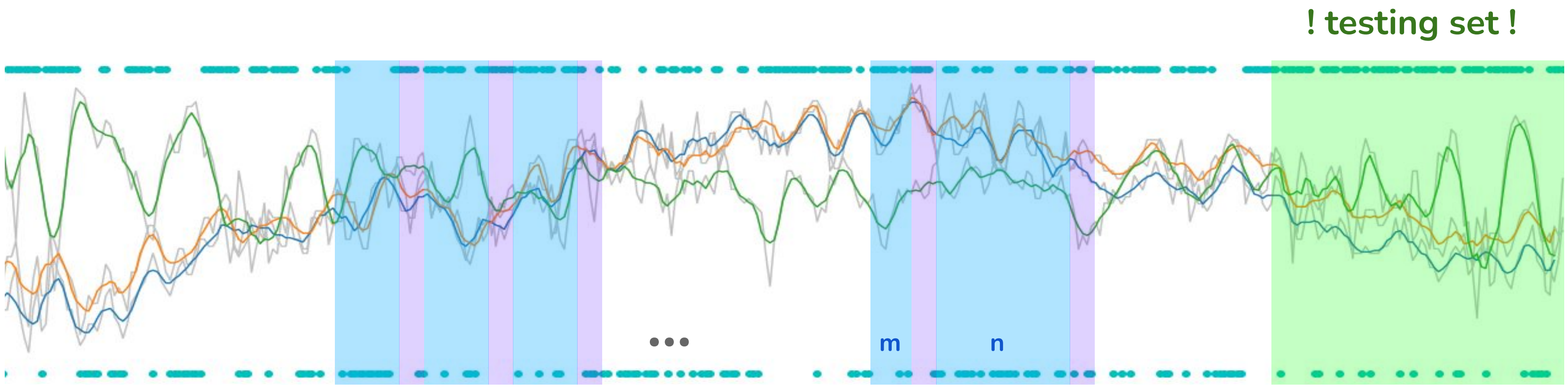
Training set construction



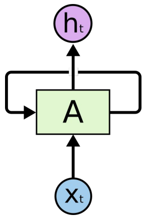


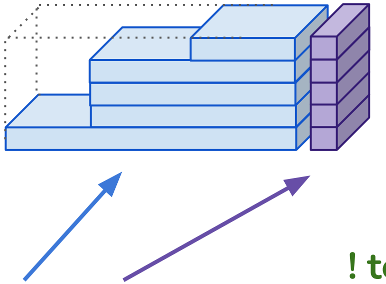
Training set construction

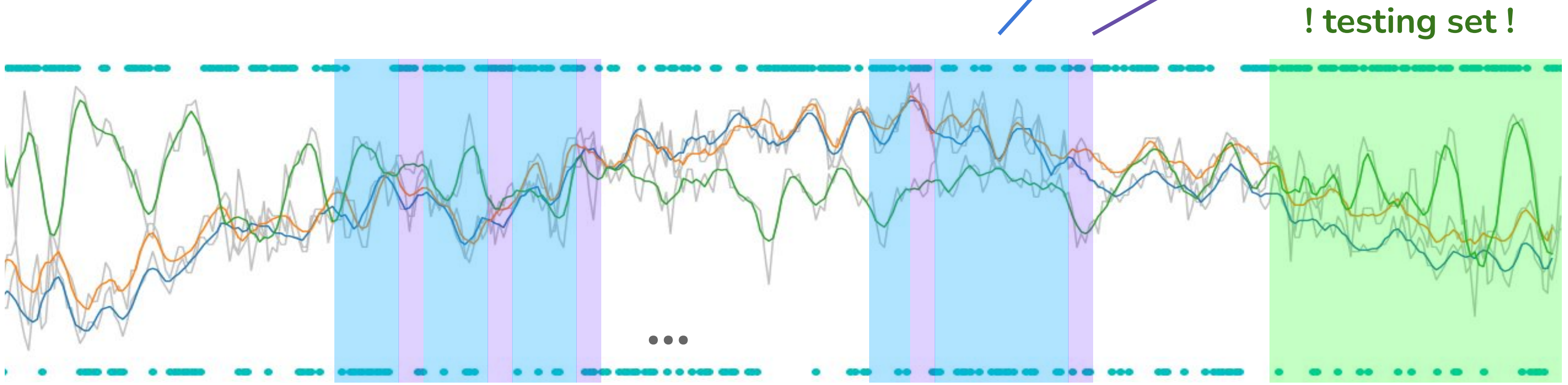




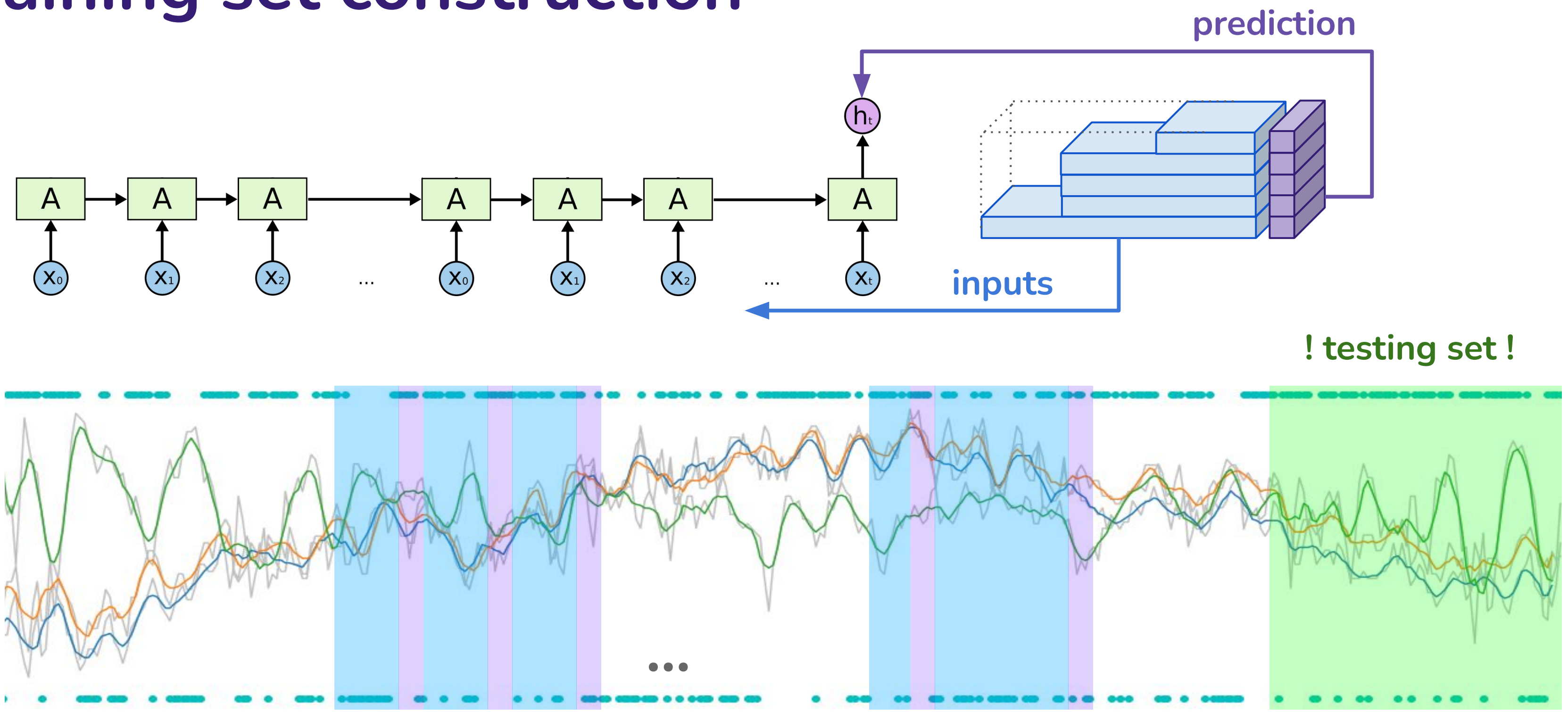
Training set construction



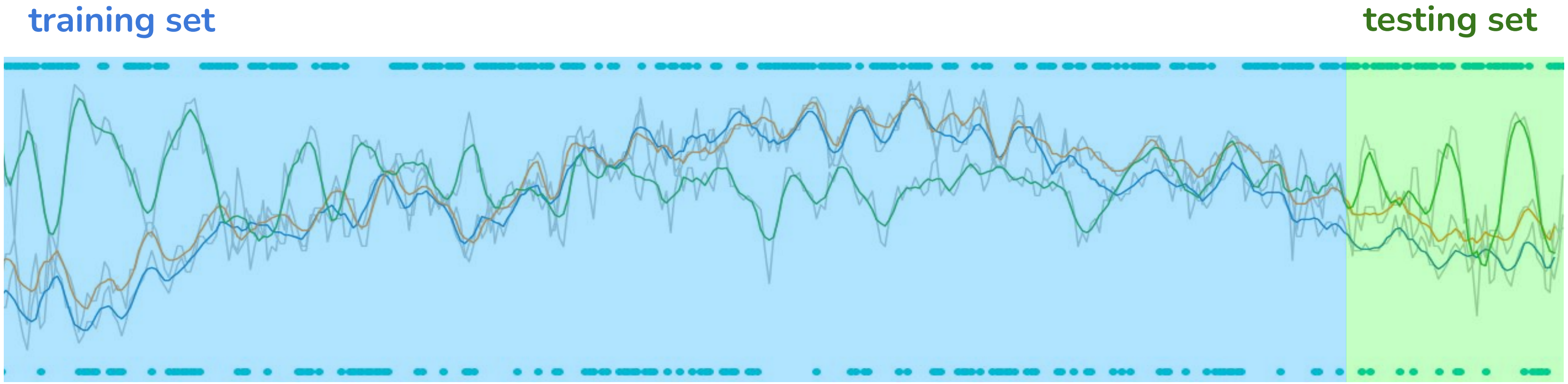




Training set construction



Training set construction



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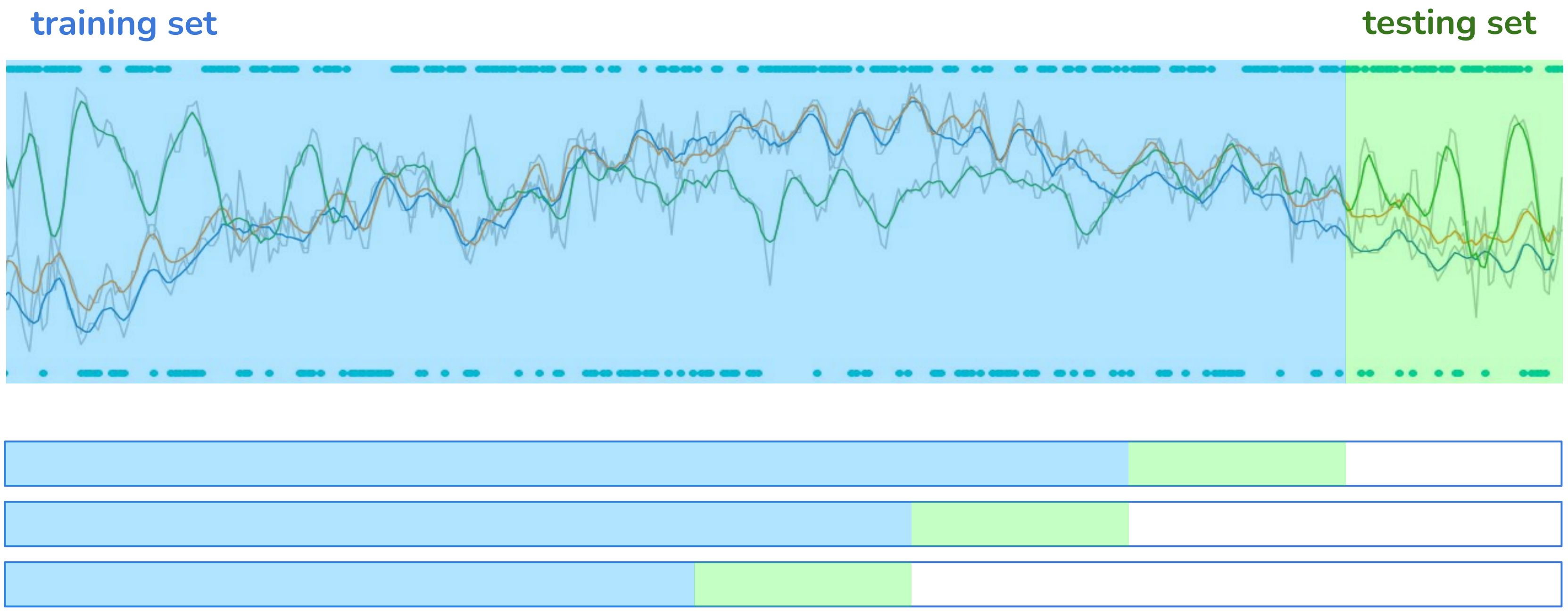

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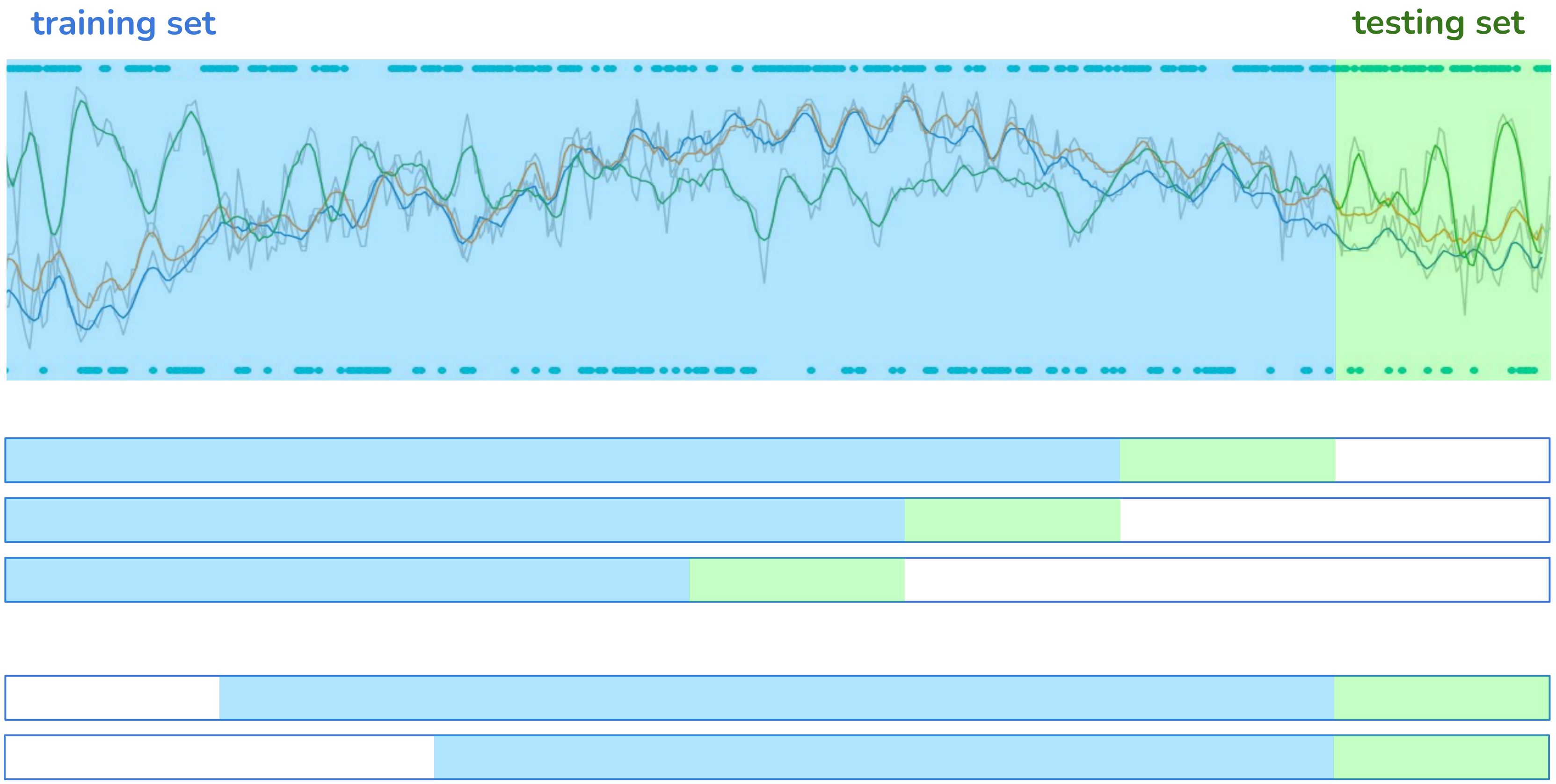
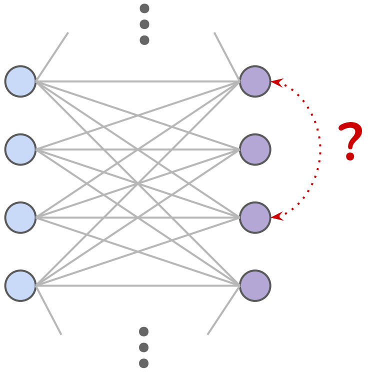


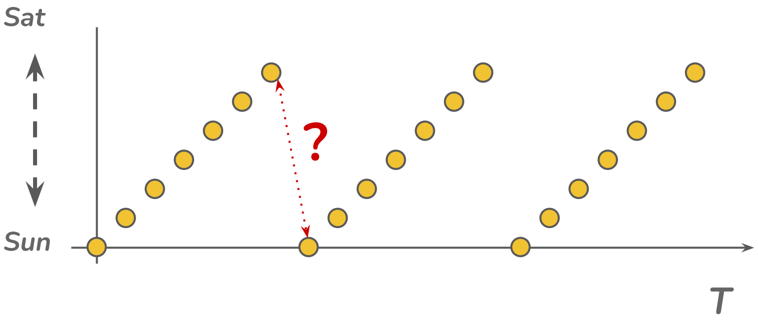
Feature Encoding – Seasonal dummy variables

- *(hour of day, day of week, ...)*
- *Numerical variables*
- *One-hot encoding*

Sun	0	0	0	0
Mon	**1**	0	0	0
Tue	0	**1**	0	0
Wed	0	0	**1**	0
Thu	0	0	0	**1**
Fri	0	0	0	0
Sat	0	0	0	0

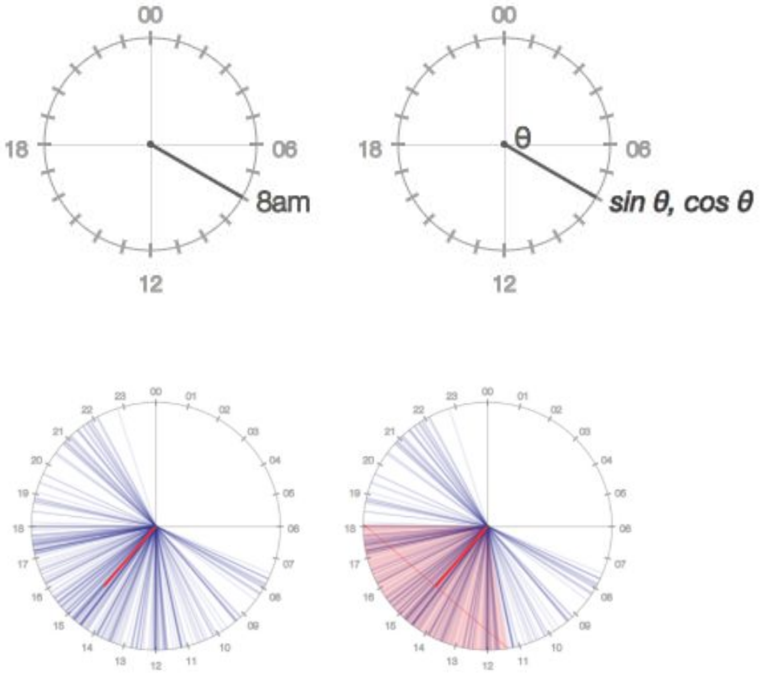
T →



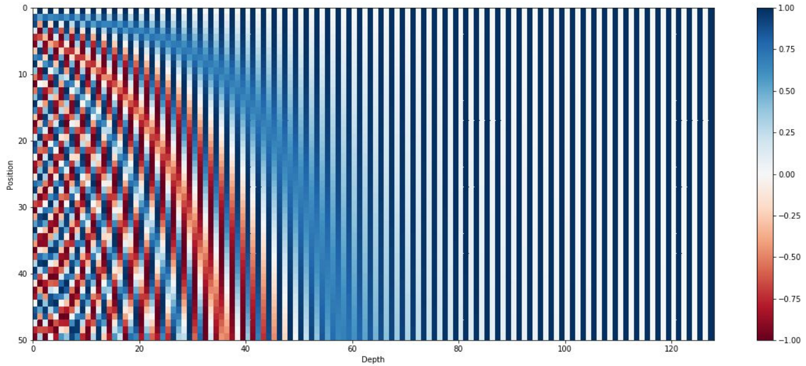


https://medium.com/life-at-hopper/ai-in-travel-part-2-representing-cyclic-and-geographic-features-4ada33dd0b22
https://kazemnejad.com/blog/transformer_architecture_positional_encoding/

Feature Encoding – Seasonal dummy variables



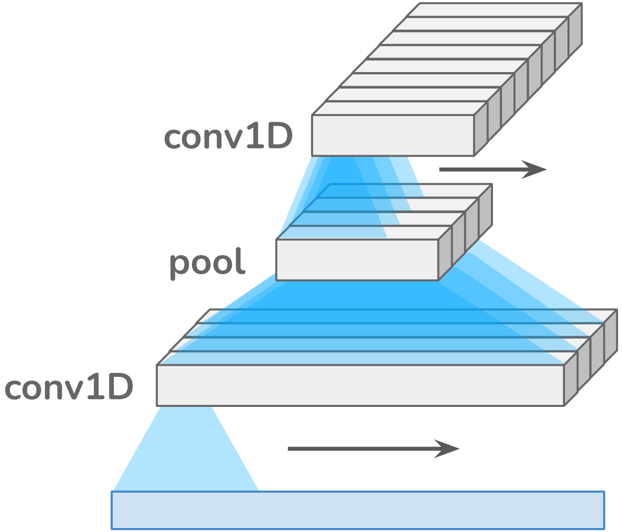
- *Circular encoding*
- *Positional embedding (transformers)*

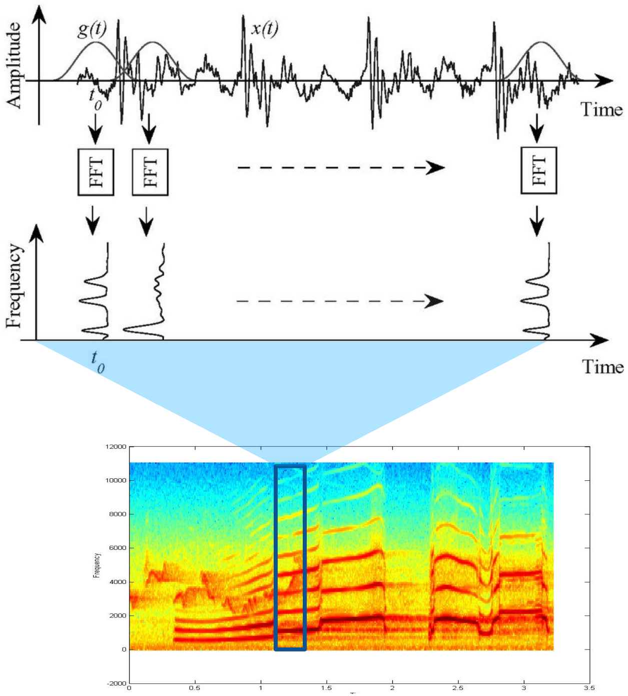


https://medium.com/life-at-hopper/ai-in-travel-part-2-representing-cyclic-and-geographic-features-4ada33dd0b22
https://kazemnejad.com/blog/transformer_architecture_positional_encoding/

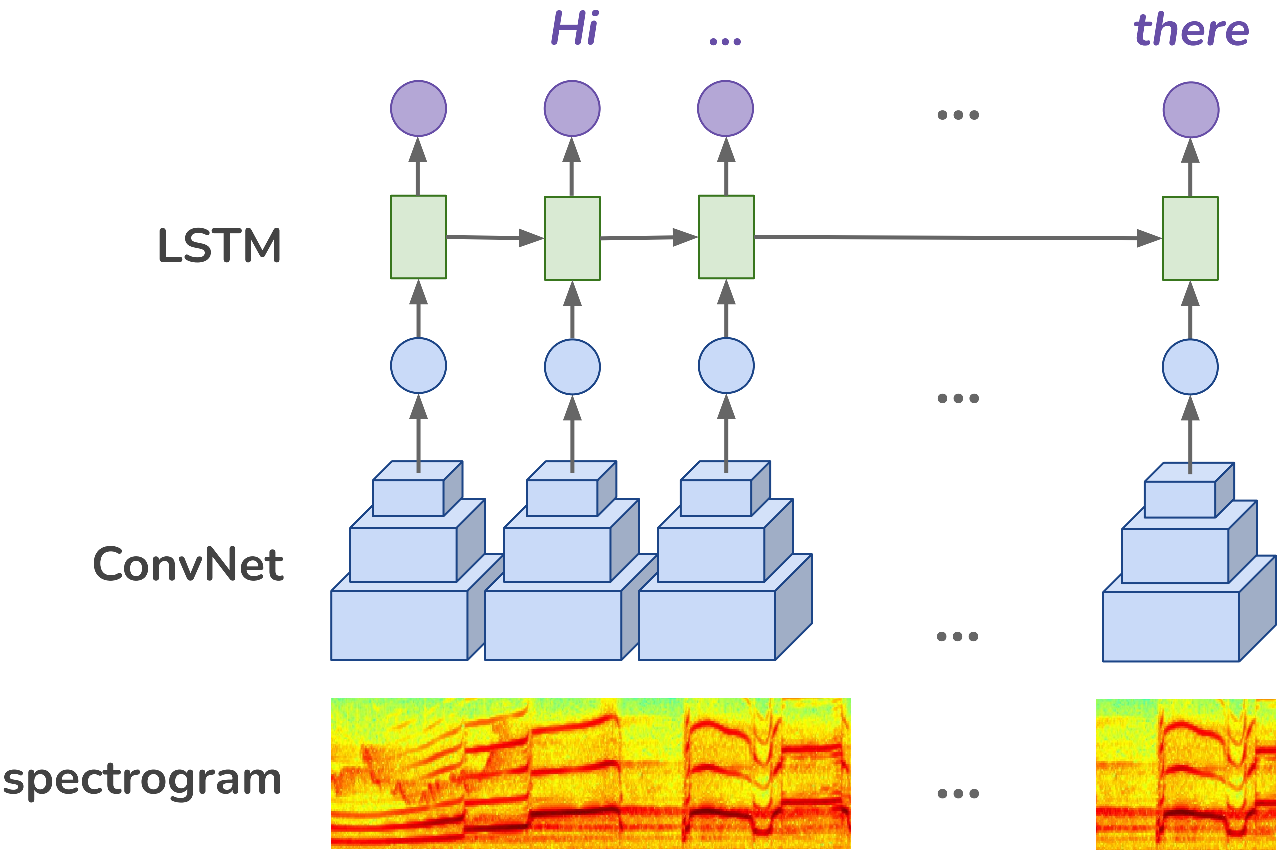
Feature Encoding II

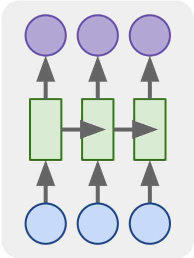
- Exchange for extra dimension
  - 1D Convolution & pooling
  - Short-Time Fourier Transform





Speech recognition





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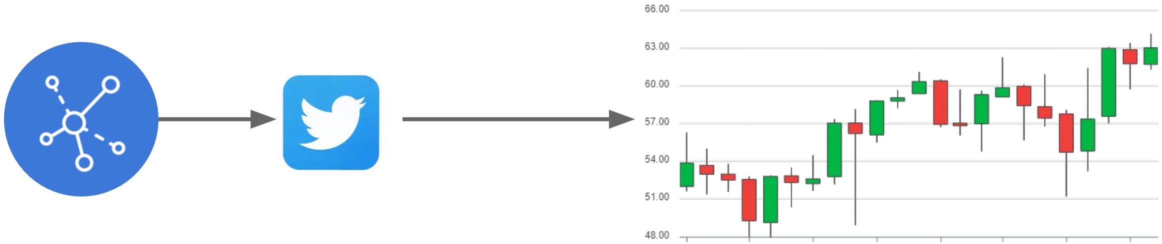
Time series prediction from textual data



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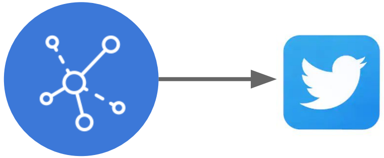
Time series prediction from textual data



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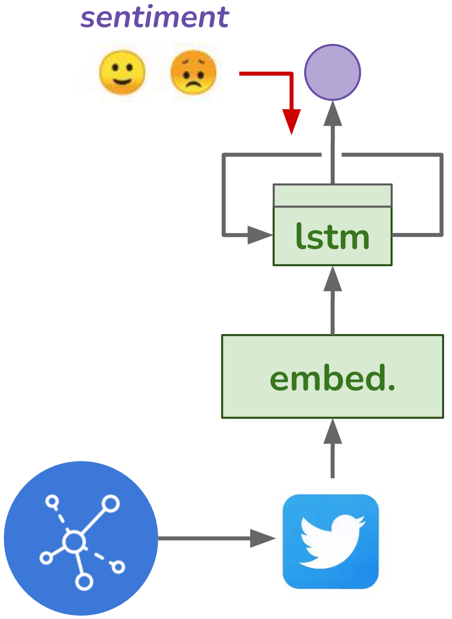
Pre-training with additional data

pre-training



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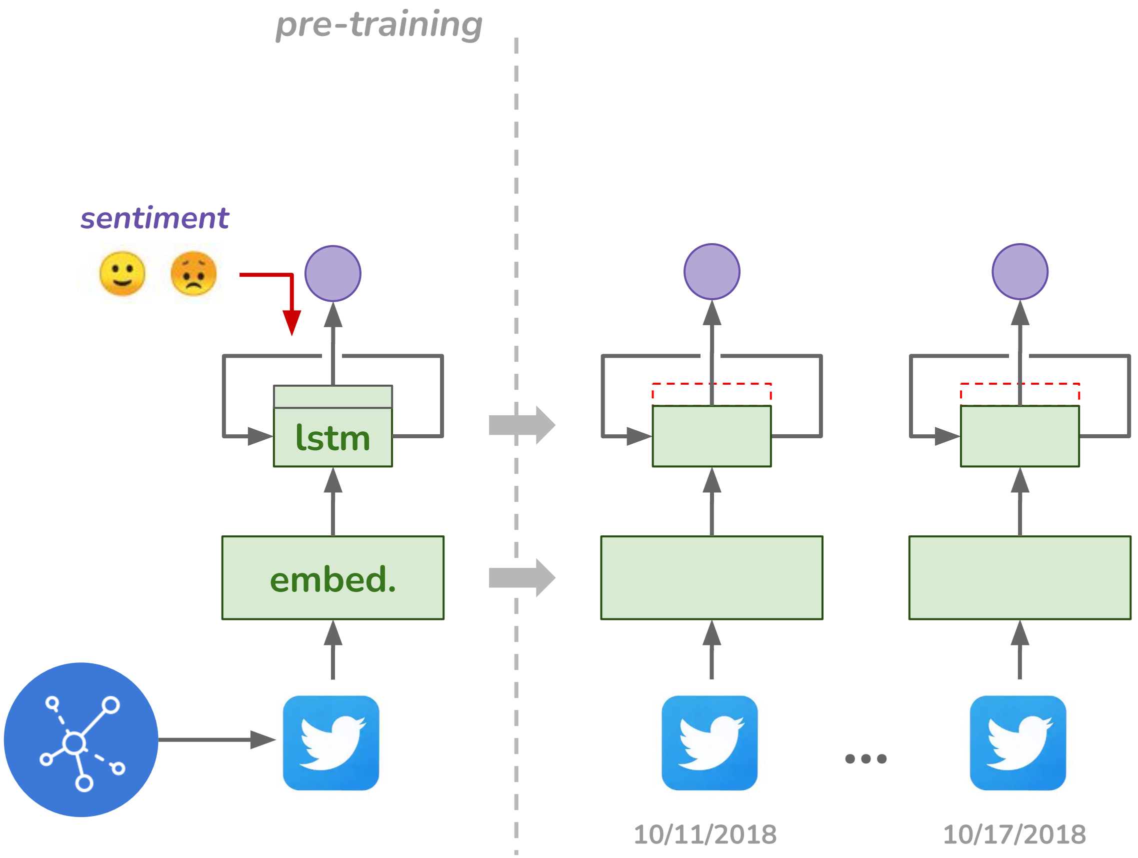
Transfering model & exposing feature layer



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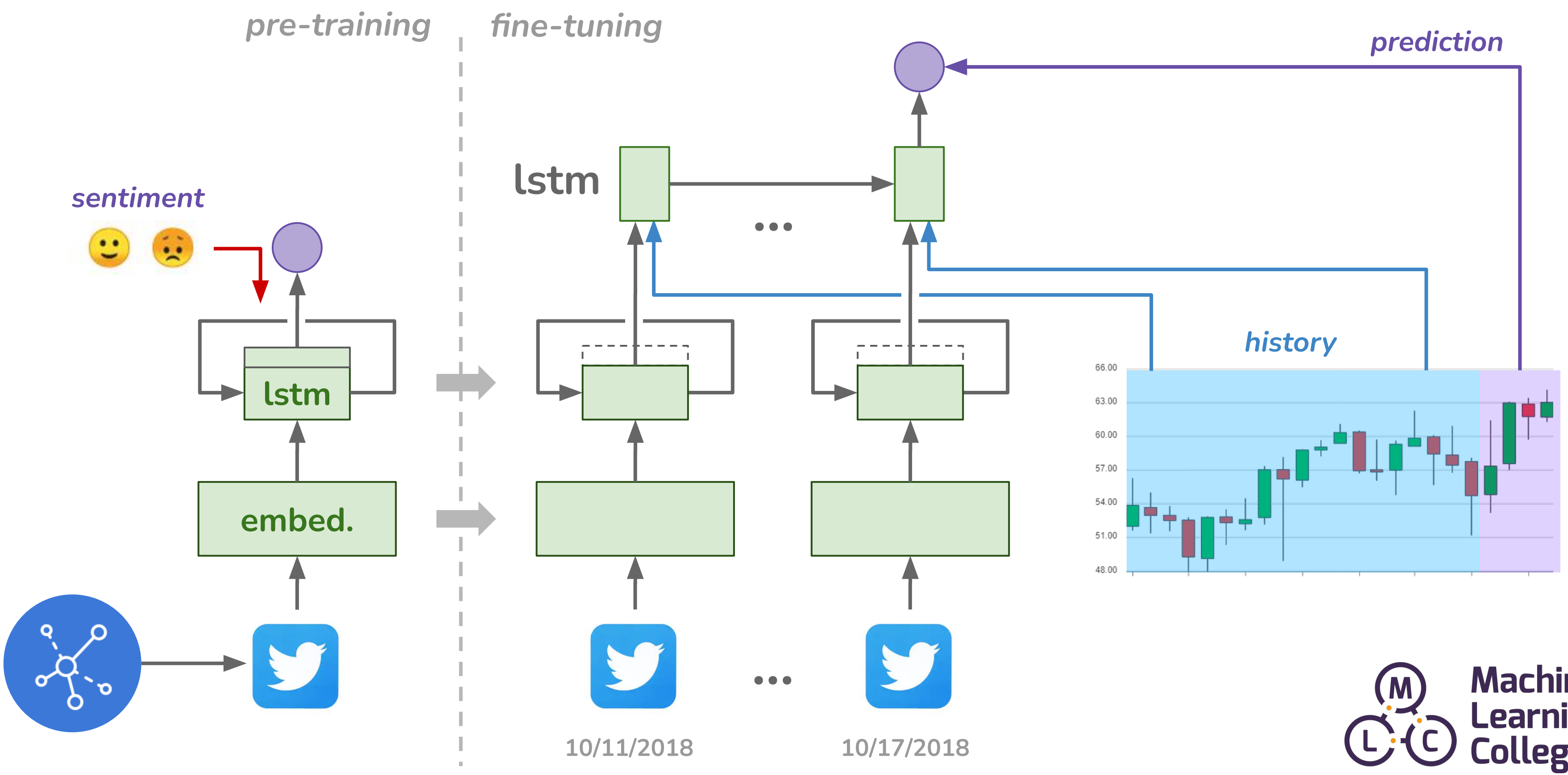
Fine-tuning with time series target data



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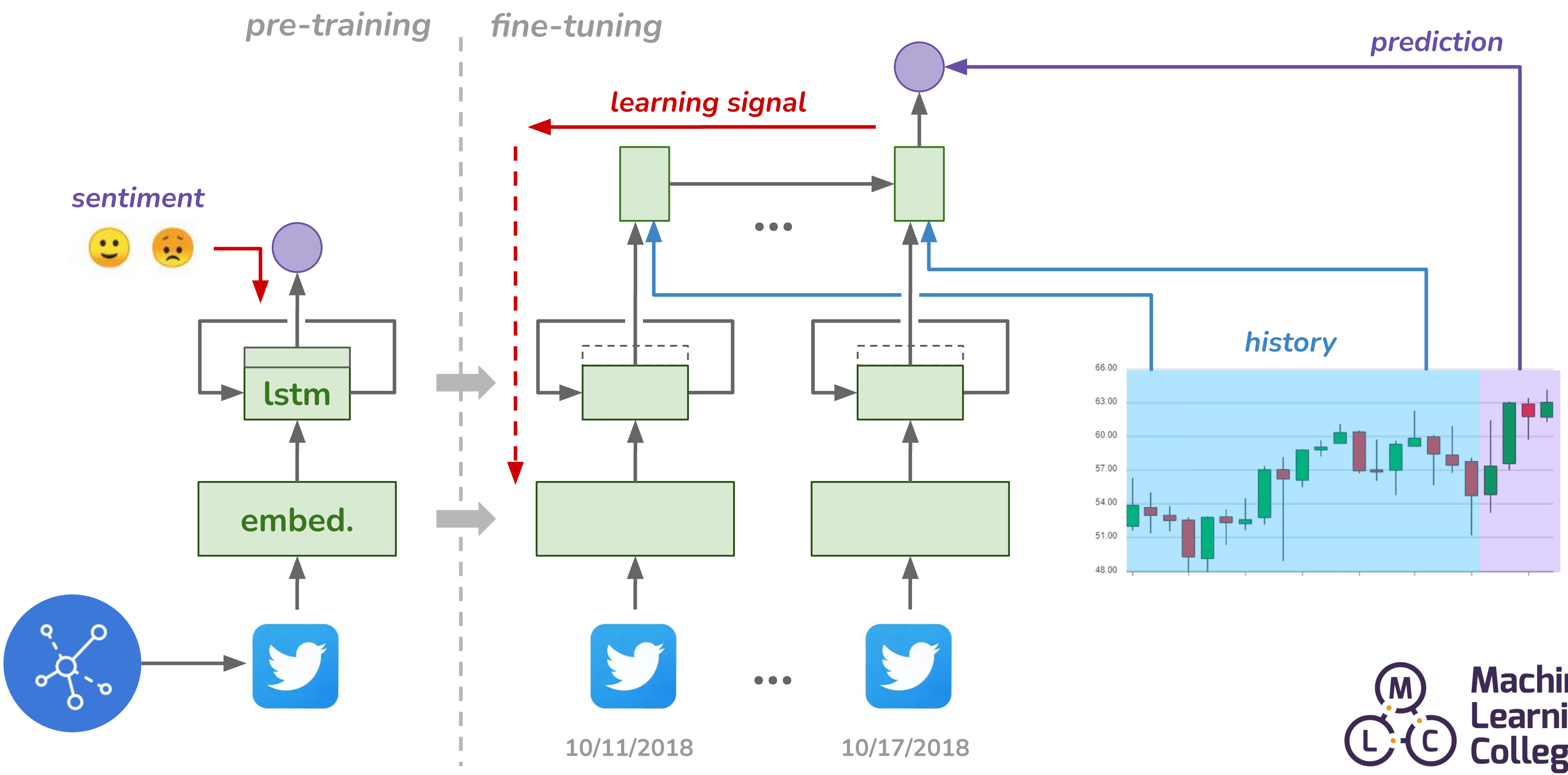

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ML & Product Design

- ML should solve problems
  - *Easily solvable by human* ⇒ scale up & automate
  - *Not easily solvable by human* ⇒ too complex or not sensitive enough
- Automation is a spectrum
  - Collaboration instead of full automation
    - No automation
    - Scored set of possible decisions
    - Narrowed set of decision to approve
    - Veto before automatic execution
    - Full automation
- Models are imperfect
  - Right evaluation metrics
  - Expectation control / Automation bias
- End-to-end models?
  - Explainability
  - Configurability

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ML Tips & Tricks

- Known your data
    - Visualize everything you can
    - Try to find patterns ⇒ *become the model yourself*
    - Look for noisy labels / missing data
    - Make sure your preprocessing is correct (especially vectorized code)
- Start with simple models
    - Build training & evaluation loop
    - Choose simple architectures first ⇒ *less room for errors*
    - Build baseline models for comparison ⇒ *even simple heuristics are useful*
- Train iteratively
    - Train without inputs ⇒ *yields another baseline model*
    - Overfit one batch ⇒ *something is off if you can't get zero loss*
    - Overfit the training set as far as you can
- Regularize
    - Early stopping ⇒ *best evaluation loss*
    - Make the model smaller ⇒ *less space for overfitting*
    - Get more training data ⇒ *more labels, data augmentation, pre-training*

http://karpathy.github.io/2019/04/25/recipe/