Time Series Modeling using Neural Networks

Dušan Fedorčák 09/2022



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)

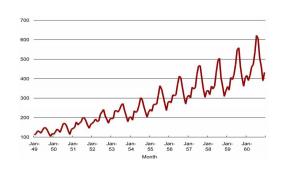
- Exoplanets Hunting
- Mobile Motion Sensing

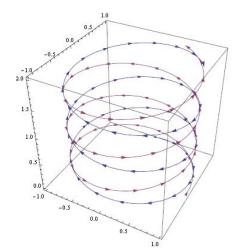
lunch break -

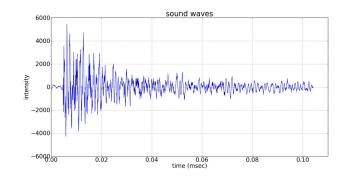
- Manufacturing Process Modeling
- Financial distress prediction
- Google Drive Folder with data
- <u>GitHub repository</u> with example sources
- this presentation



Time series – example data



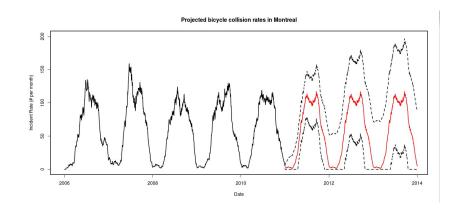


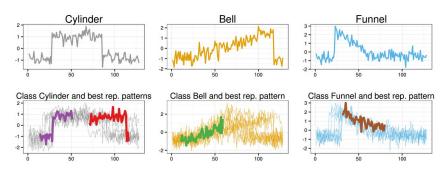


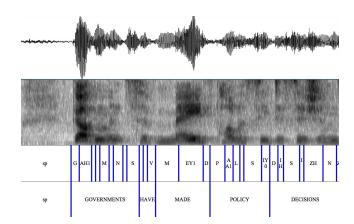


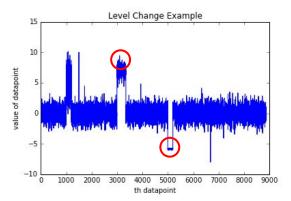


Time series – example tasks





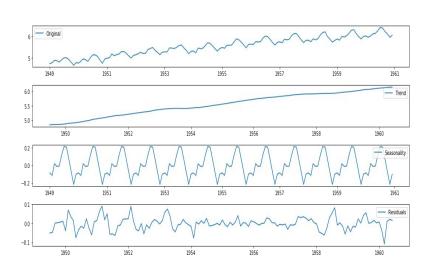


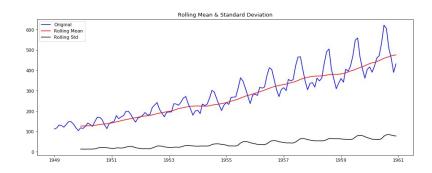


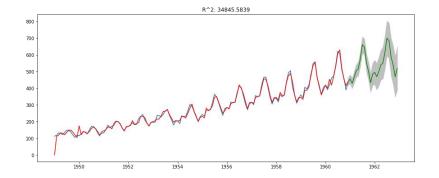


Time Series – classical analysis & modeling

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









Time Series – classical analysis & modeling

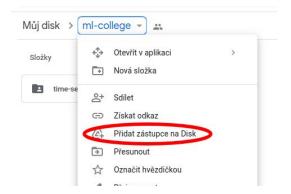
1. Open this link

or

- 1. Open colab.google.com
- 2. In the Open Notebook menu
 - a. Navigate to GitHub tab
 - b. Enter **mlcollege** into search bar
 - c. Select mlcollege/timeseriesanalysis repo
 - d. Open arima-complete.ipynb

Do not forget to add this

<u>Google Drive Folder</u> to your
drive





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
 - State Equation
 - $\mathbf{x}_{t} = \mathbf{F}\mathbf{x}_{t-1} + N(0, \mathbf{Q})$ sometimes without noise
 - Observation Equation

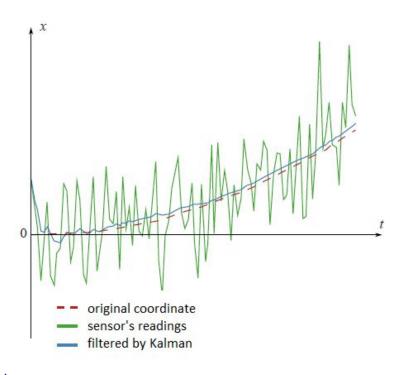


Kalman Filter

- Evolve state
 - $x'_t = Fx_{t-1}$ $P'_t = FP_{t-1}F^T + Q$
- Integrate observation

$$\circ \quad \mathbf{P_t} = (\mathbf{I} - \mathbf{K_t} \mathbf{H}) \; \mathbf{P'_t}$$

- Kalman Gain
 - $\circ K_t = P'_t H^T (HP'_t H^T + R)^{-1}$
- ARIMA and Kalman Filter
 - ARIMA can be viewed as a state space model
 - ARIMA can be fitted with MLE via Kalman Filter
 - o https://bookdown.org/rdpeng/timeseriesbook/maximum-likelihood-with-the-kalman-filter.html
 - https://towardsdatascience.com/the-kalman-filter-and-maximum-likelihood-9861666f6742





Hidden Markov Model

- Model Description
 - \circ HMM (λ) can be viewed as a state space model
 - Finite set of hidden states

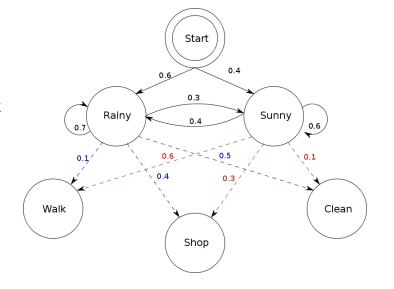
•
$$\mathbf{Q} = \{q_1, q_2, ..., q_n\}, \ \boldsymbol{\pi} = \{\pi_1, \pi_2, ..., \pi_n\} - \text{init}$$

- \mathbf{n} number of states (hyperparameter)
- Set of observations

$$\mathbf{O}_{i} = (o^{1}, o^{2}, o^{3}, ..., o^{T})$$

Transition probability matrix & emissions

■
$$A = (a_{00}, ..., a_{nn}), B = q_i \rightarrow 0$$



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



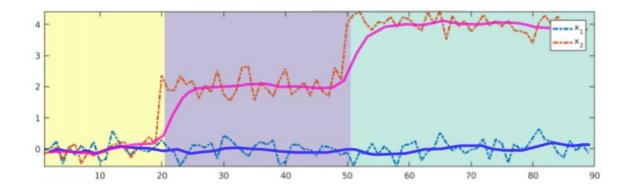
Kalman Filter vs. Hidden Markov Model

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





Time Series – goals 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

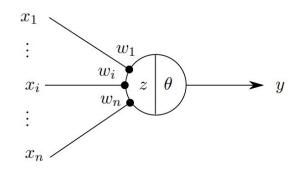
Given a complete dataset, what can I infer about the true state of nature in the past?

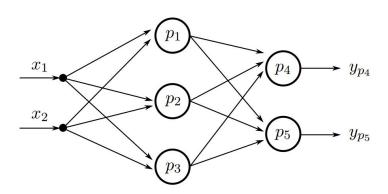
Regression

Given a time series of two phenomena, what is the association between them?



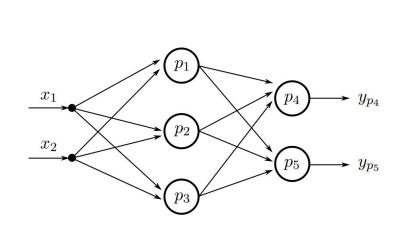
Neural networks

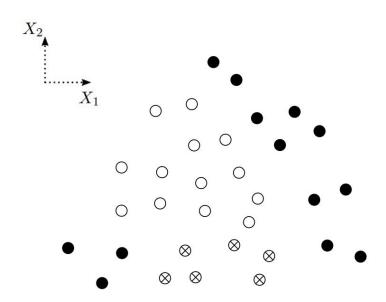




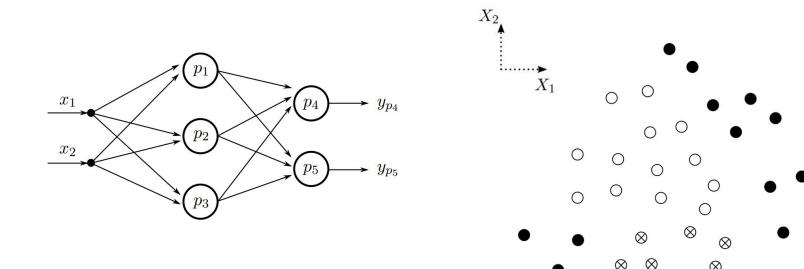
- Artificial Neural Cells
 - Linear combination of inputs
 - Non-linear activation function
- Connected Neurons
 - Directed graph
 - Layered structure
 - Dense connections
 - Convolutions & pooling
 - Recurrency, signal gates
 - Masking & attention heads
- Universal function approximator
 - Trainable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





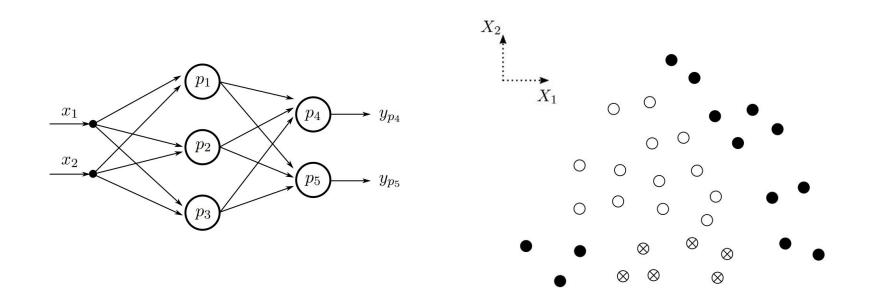






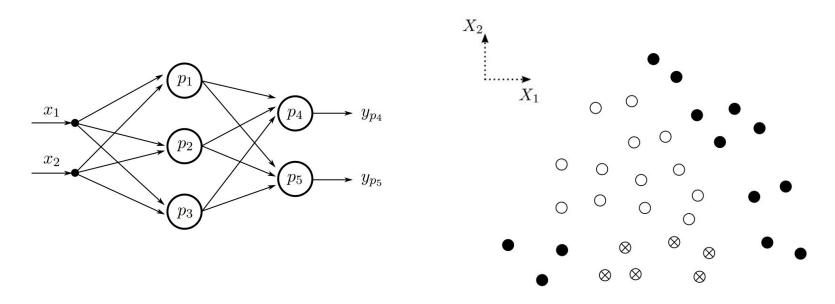
$$y = s(\sum w_i x_i - \theta)$$





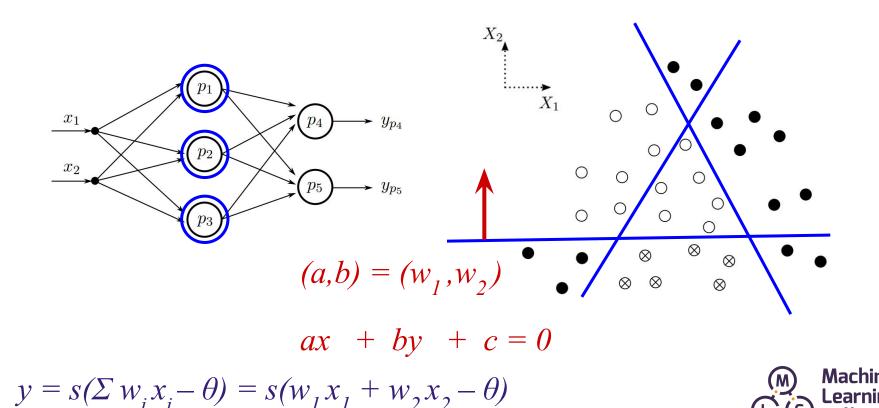
$$y = s(\Sigma w_i x_i - \theta) = s(w_1 x_1 + w_2 x_2 - \theta)$$

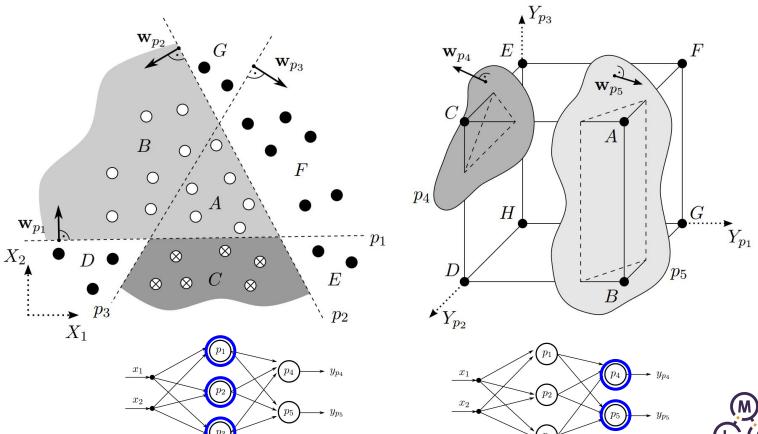




$$ax + by + c = 0$$
$$y = s(\sum w_{i}x_{i} - \theta) = s(w_{1}x_{1} + w_{2}x_{2} - \theta)$$

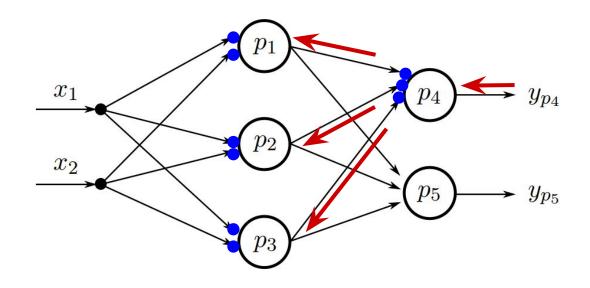






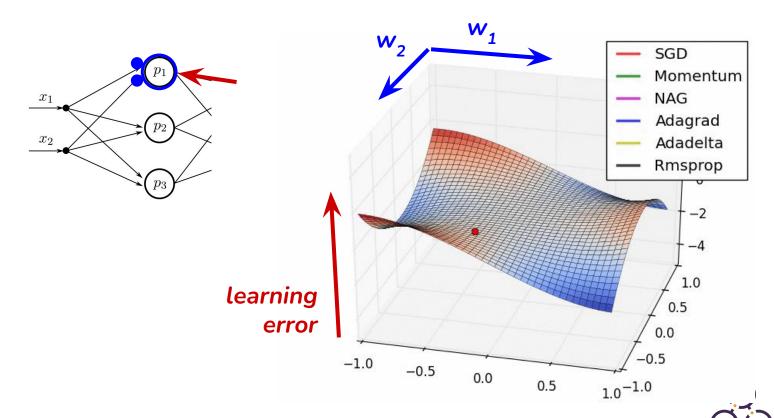
Machine

Neural networks – Backpropagation





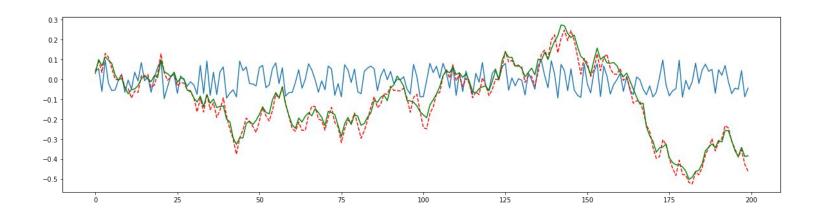
Neural networks - Backpropagation



Machine

Learning College

Time Series with Neural Networks

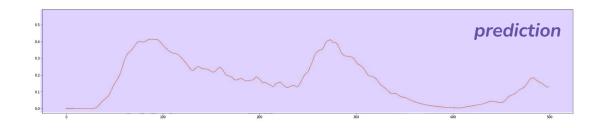


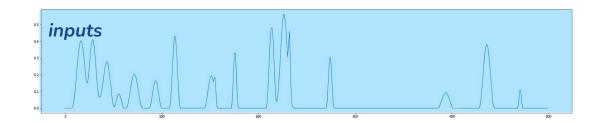
Neural Networks

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

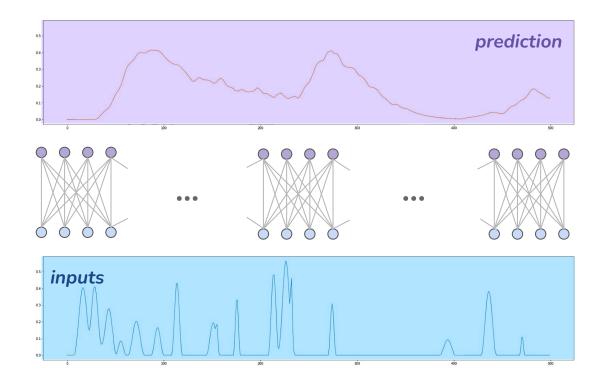


How neural network fits?

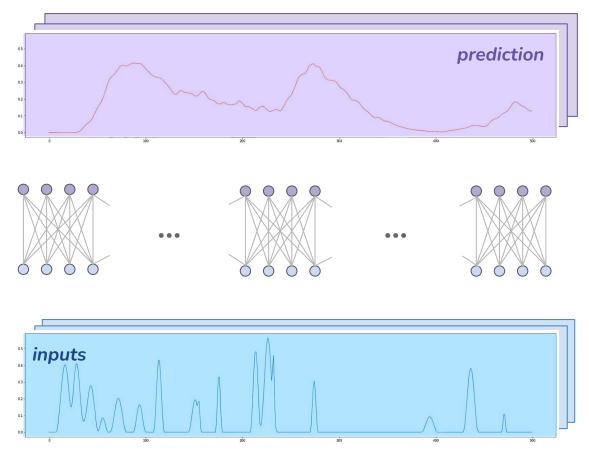




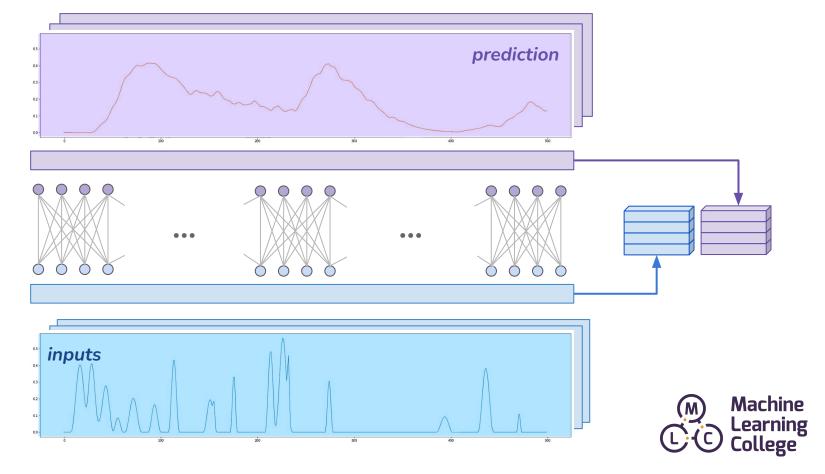


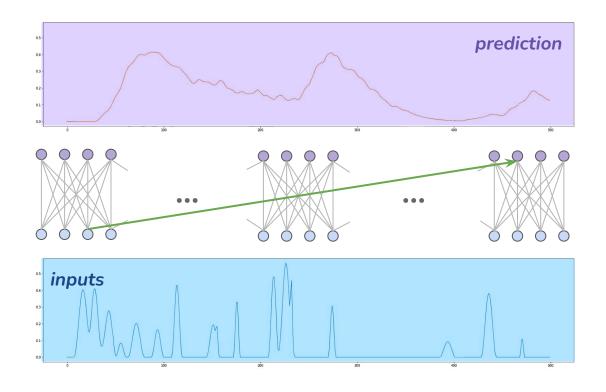




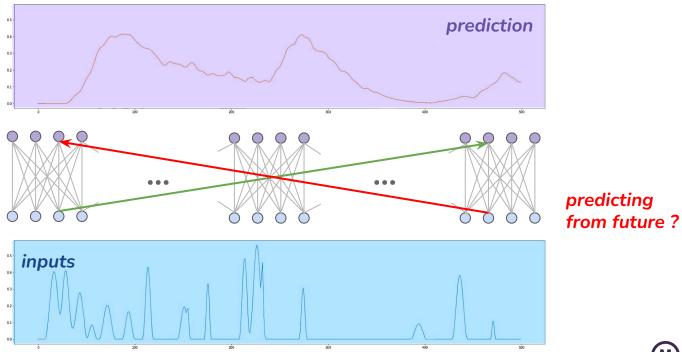




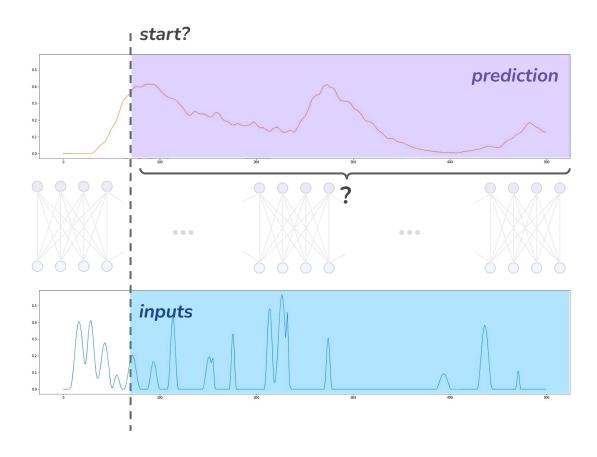




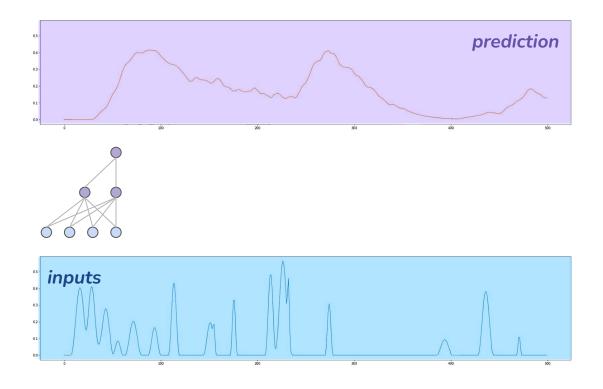




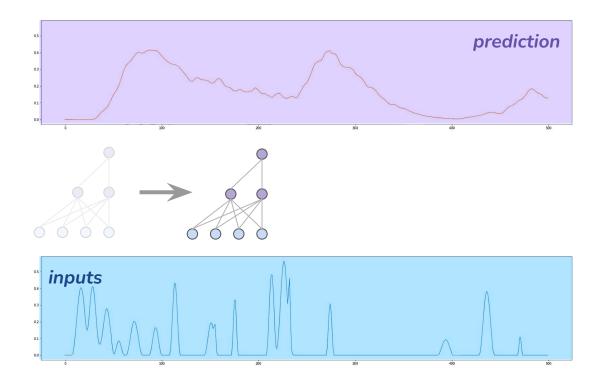




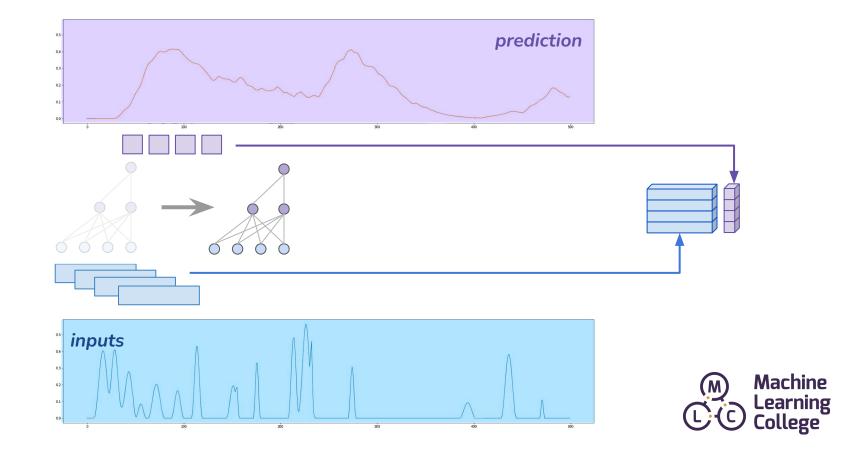


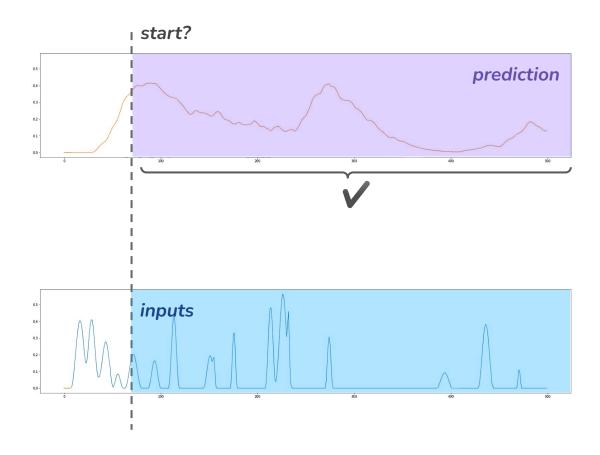




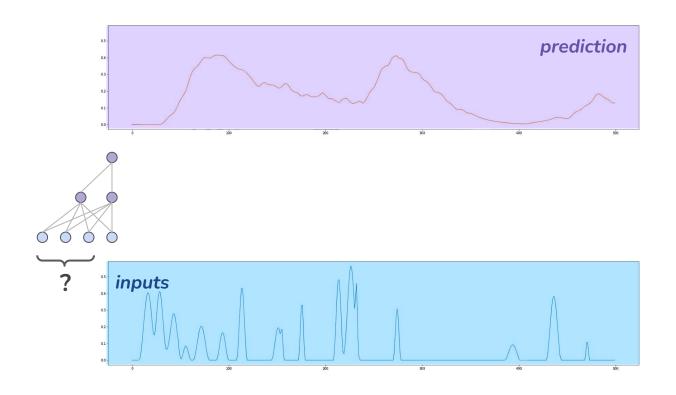




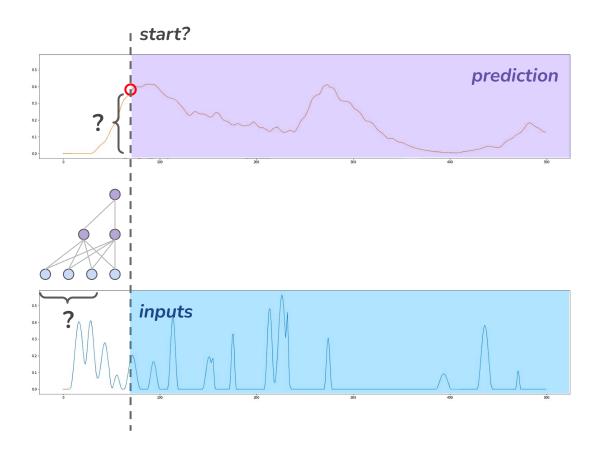






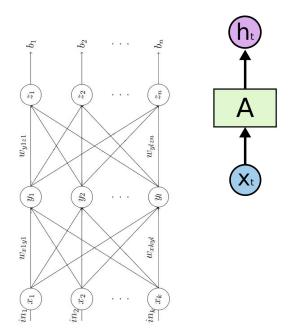


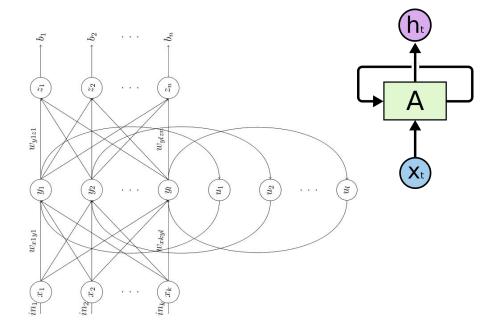




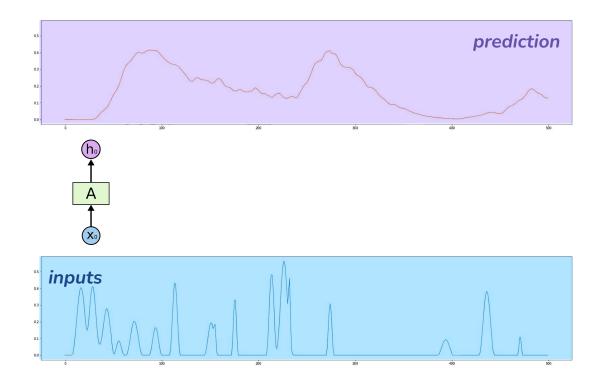


Recurrent Neural Networks





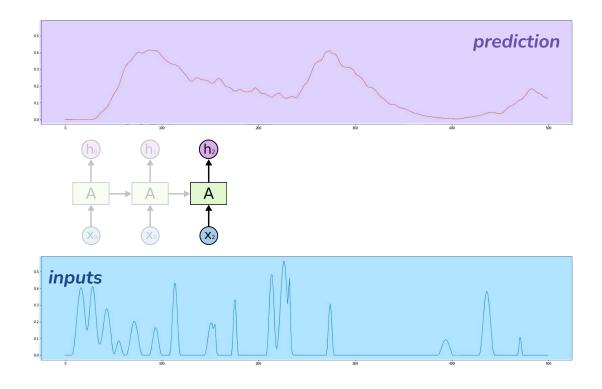




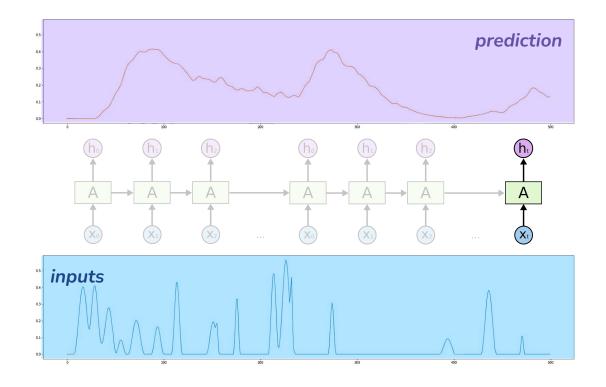




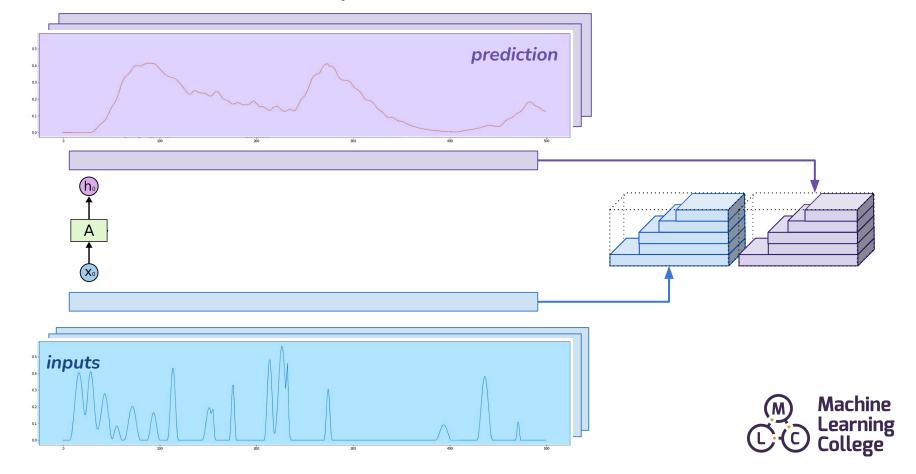


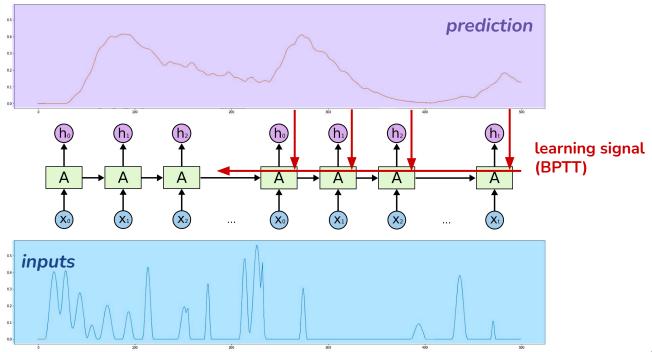






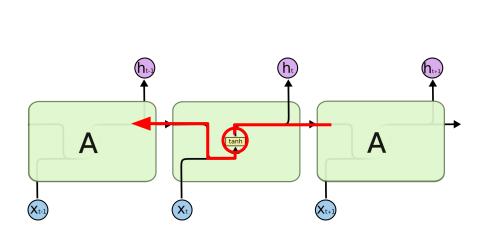


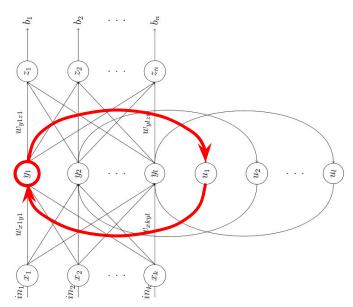






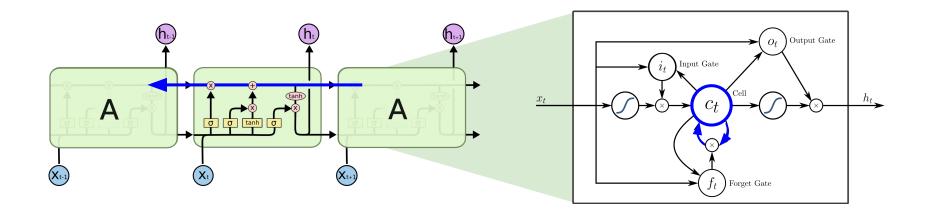
RNN – Vanishing gradients



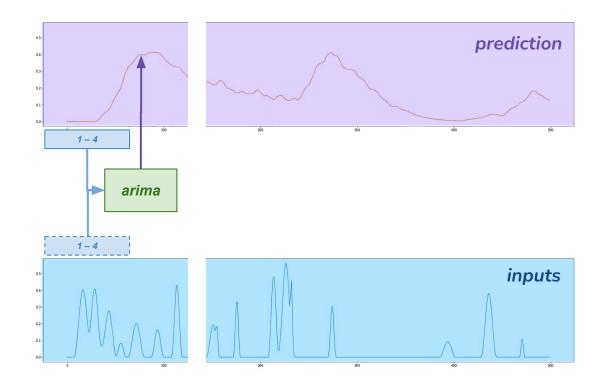




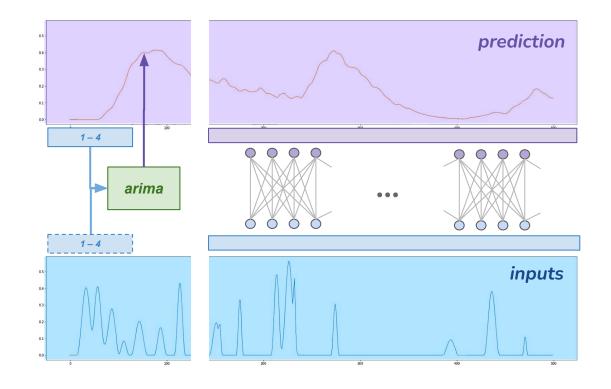
Long short-term memory – LSTM



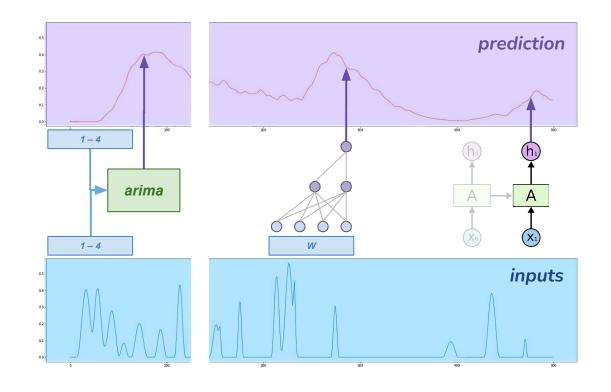




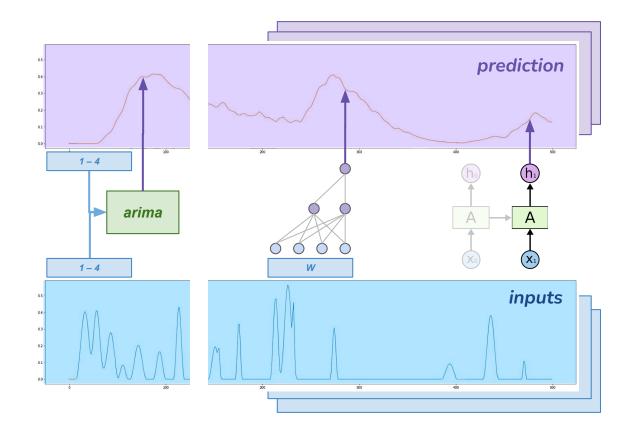






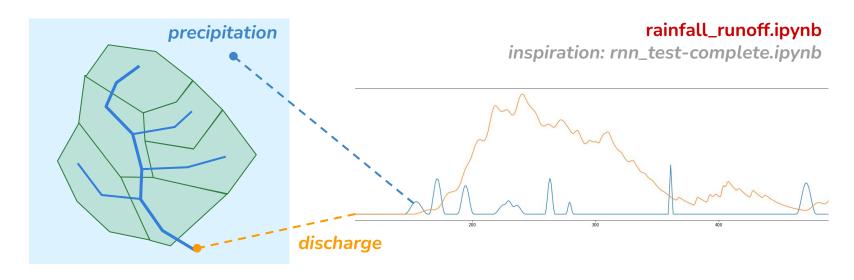








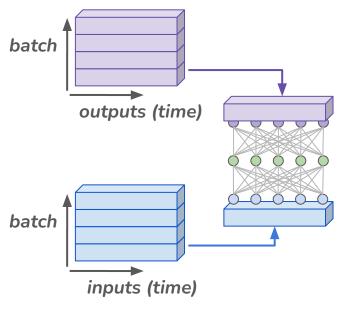
Rainfall-runoff example



- 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



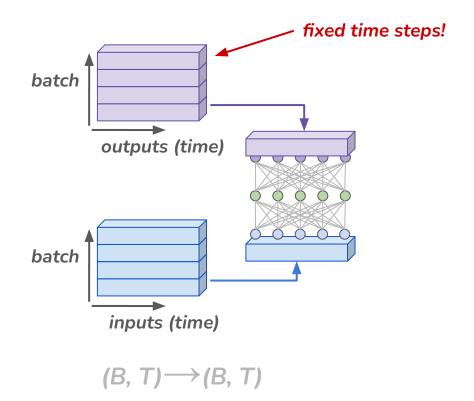
Flat NN = 2D training data





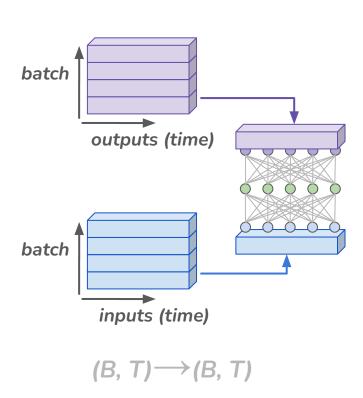


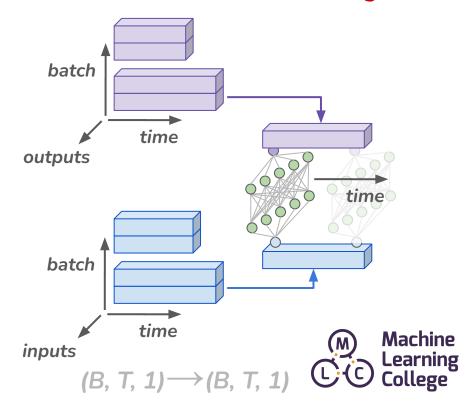
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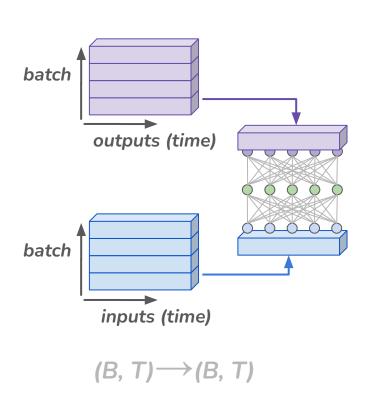


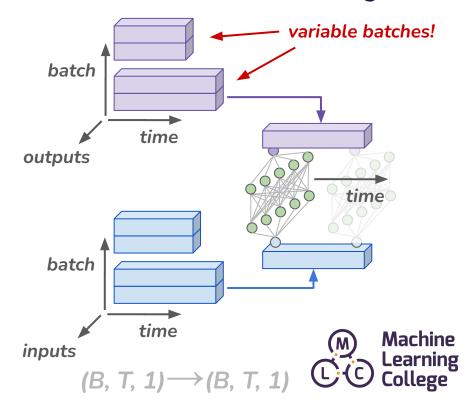
Flat NN = 2D training data





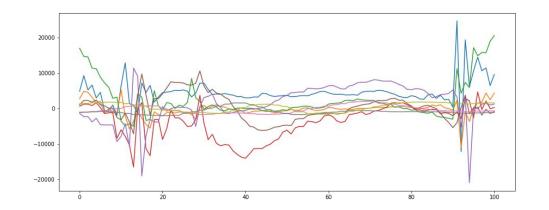
Flat NN = 2D training data





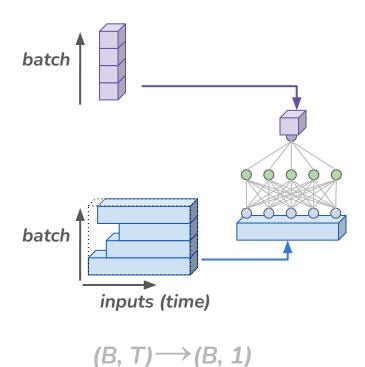
Trampoline jumping example

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





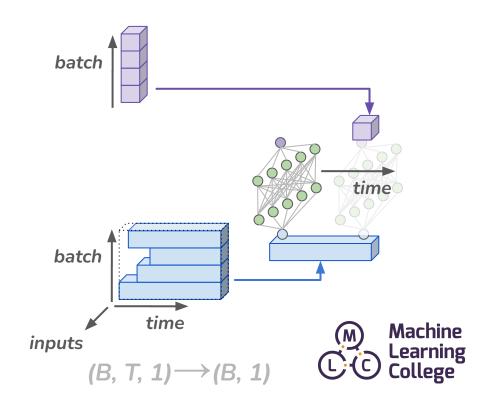
Flat NN = 2D training data





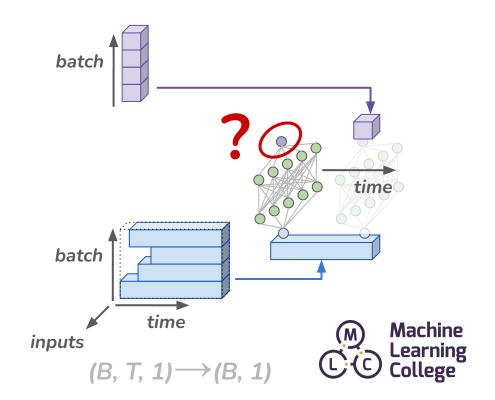
Flat NN = 2D training data

batch batch inputs (time)



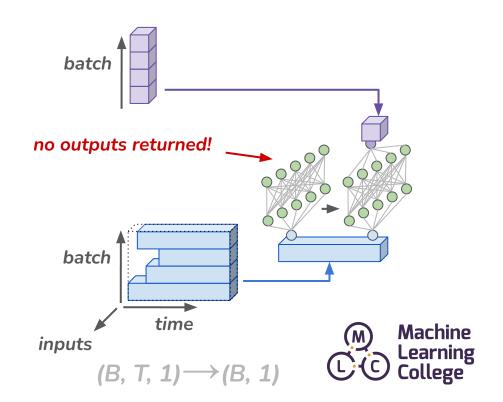
Flat NN = 2D training data

batch batch inputs (time)



Flat NN = 2D training data

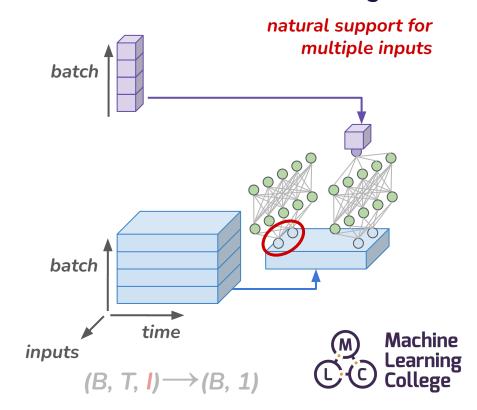
batch batch inputs (time)



Tensors & dimentions – multivariate b. classification

Flat NN = 2D training data

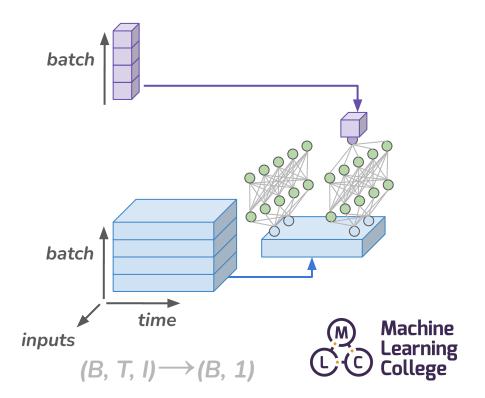
?



Tensors & dimentions – multivariate b. classification

Flat $NN = 3D \rightarrow 2D$ training data

flattening / interleaving batch outputs batch time inputs $(B, \mathsf{T} \times \mathsf{I}) \longrightarrow (B, \mathsf{T} \times \mathsf{O})$

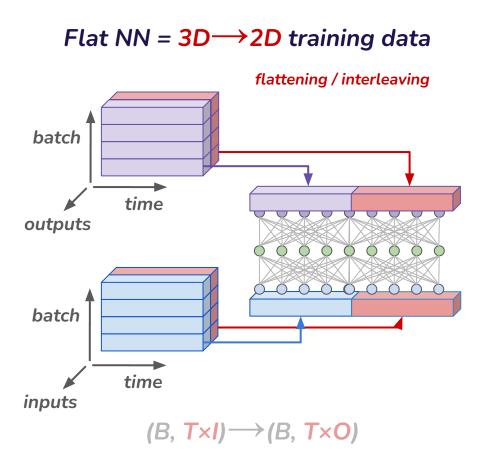


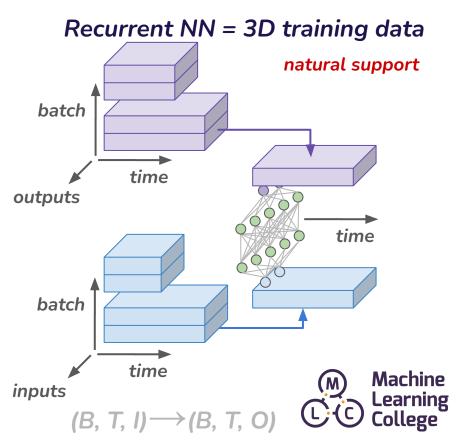
Binary classification – confusion matrix

		Predicted condition		Sources: [20][21][22][23][24][25][26][27] view+talk+edit	
	Total population = P + N	Positive (PP)	Negative (PN)	Informedness, bookmaker informedness (BM) = TPR + TNR - 1	Prevalence threshold (PT) = \frac{\sqrt{TPR \times FPR}}{TPR - FPR}
condition	Positive (P)	True positive (TP),	False negative (FN), type II error, miss, underestimation	True positive rate (TPR), recall, sensitivity (SEN), probability of detection, hit rate, power $= \frac{TP}{P} = 1 - FNR$	False negative rate (FNR), miss rate = $\frac{FN}{P} = 1 - TPR$
Actual c	Negative (N)	False positive (FP), type I error, false alarm, overestimation	True negative (TN),	False positive rate (FPR), probability of false alarm, fall-out $= \frac{FP}{N} = 1 - TNR$	True negative rate (TNR), specificity (SPC), selectivity = $\frac{TN}{N} = 1 - FPR$
	Prevalence $= \frac{P}{P+N}$	Positive predictive value (PPV), precision $= \frac{TP}{PP} = 1 - FDR$	False omission rate (FOR) $= \frac{FN}{PN} = 1 - NPV$	Positive likelihood ratio (LR+) = TPR FPR	Negative likelihood ratio (LR-) $= \frac{FNR}{TNR}$
	Accuracy (ACC) $= \frac{TP + TN}{P + N}$	False discovery rate (FDR) $= \frac{FP}{PP} = 1 - PPV$	Negative predictive value (NPV) $= \frac{TN}{PN} = 1 - FOR$	Markedness (MK), deltaP (Δp) = PPV + NPV - 1	Diagnostic odds ratio (DOR) = $\frac{LR+}{LR-}$
	Balanced accuracy (BA) $= \frac{TPR + TNR}{2}$	$F_1 \text{ score}$ $= \frac{2PPV \times TPR}{PPV + TPR} = \frac{2TP}{2TP + FP + FN}$	Fowlkes–Mallows index (FM) = √PPV×TPR	Matthews correlation coefficient (MCC) = √TPR×TNR×PPV×NPV - √FNR×FPR×FOR×FDR	Threat score (TS), critical success index (CSI),

https://en.wikipedia.org/wiki/Confusion_matrix







Time Series Modeling using Neural Networks – DAY 2

Dušan Fedorčák 02/2022 – 02



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
- Practical Examples (in random order)
 - Exoplanets Hunting
 - Mobile Motion Sensing
 - lunch break –
- Tips & tricks for debuging NNs
- Practical Examples
 - Manufacturing Process Modeling
 - Financial distress prediction



ML & Product Design – problems & decisions

- ML should solve problems
 - Al is cool ⇒ let's use it in the product! *
 - We need to solve this problem \Rightarrow can we apply ML? \checkmark
 - Q: What other means of solving the problem are available?



ML & Product Design – problems & decisions

- ML should solve problems
 - Al is cool ⇒ let's use it in the product! *
 - We need to solve this problem ⇒ can we apply ML?
 - Q: What other means of solving the problem are available?
- Problems vary in difficulty
 - \circ Easily solvable by human \Rightarrow ML helps to scale up & automate
 - spam filter, face recognition, driving a car
 - \circ Not easily solvable by human \Rightarrow ML can bring some solution
 - weather forecast, stock market prediction
 - Q: What are we optimizing for? (costs, risk reduction, better service, ...)



ML & Product Design – problems & decisions

- ML should solve problems
 - Al is cool ⇒ let's use it in the product! *
 - \circ We need to solve this problem \Rightarrow can we apply ML? \checkmark
 - Q: What other means of solving the problem are available?
- Problems vary in difficulty
 - \circ Easily solvable by human \Rightarrow ML helps to scale up & automate
 - spam filter, face recognition, driving a car
 - \circ Not easily solvable by human \Rightarrow ML can bring some solution
 - weather forecast, stock market prediction
 - Q: What are we optimizing for? (costs, risk reduction, better service, ...)
- Problems boils down to decisions
 - ML can assist with decisions
 - ML can automate decisions
 - Q: Could assistance model work for us or full automation is needed?



ML & Product Design – automation

- ML solutions are imperfect
 - Expectation control & automation bias ⇒ trust issues
 - Scaling up implerfect models ⇒ quality issues
 - Right evaluation metrics model evaluation vs. UX evaluation
 - Q: Do all involved parties understand the problem & solution?
 - Q: Is there an evaluation metric everybody understands and agrees with?



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- Assistance
 ⇔ Automation there is a spectrum
 - 1. No automation
 - 2. Scored set of possible decisions
 - 3. Narrowed set of decision to approve
 - 4. Veto before automatic execution
 - 5. Full automation
 - Q: What is the lowest level of automation that brings value



ML & Product Design – data analysis

- ML solutions depends on data
 - More complex models ⇒ more data required
 - Constant battle agaings overfitting
 - Distributions shift over time
 - Q: What data is available and will be available in the future



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 - Base rates can have unintuitive effects on the product
 - Sampling reality often produces imbalanced data
 - Q: What would be the performace of near-perfect model given the base rates



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All datasets are biased

- Inconsistency between data sampling and model goals
- Biased evaluation sets
- Q: Does our historical data reliably capture the goal of the model

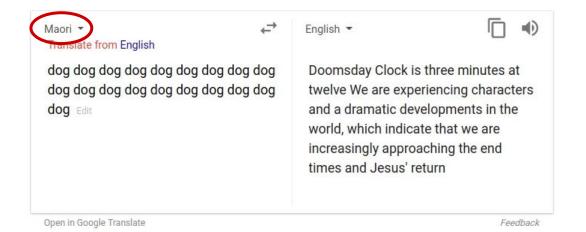


Dataset issues – insufficient number of samples

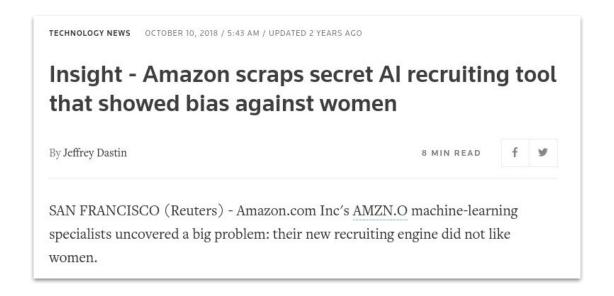




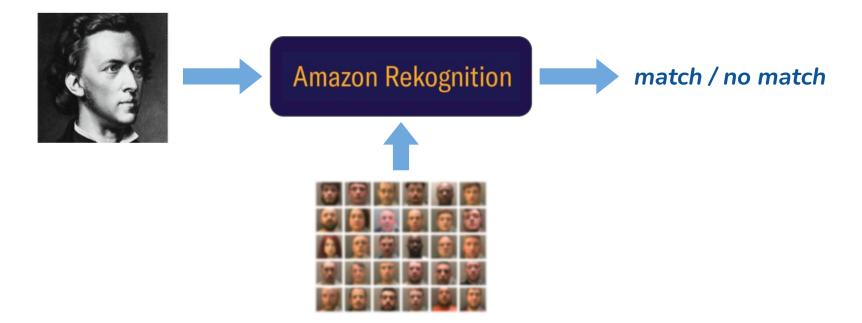
Dataset issues – insufficient number of samples







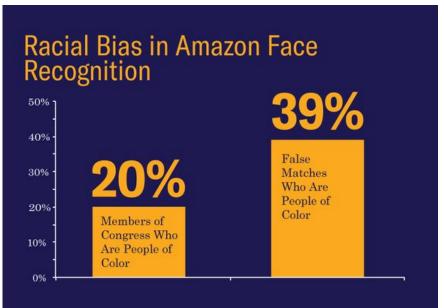














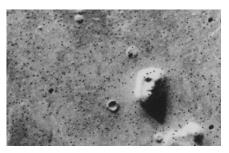
Human perception – overfitted to faces











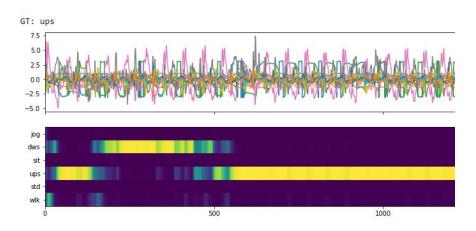






Motion sensing example

- 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







- 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)



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- Choose simple architectures first ⇒ less room for errors
- Build baseline models for comparison ⇒ even simple heuristics are useful



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- Overfit one batch ⇒ something is off if you can't get zero loss
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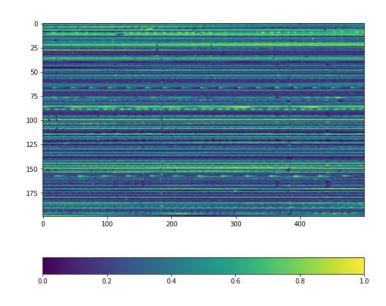
Regularize

- Early stopping ⇒ best evaluation loss
- Make the model smaller ⇒ less space for overfitting
- Get more training data ⇒ more labels, data augmentation, pre-training



Exoplanets hunting example

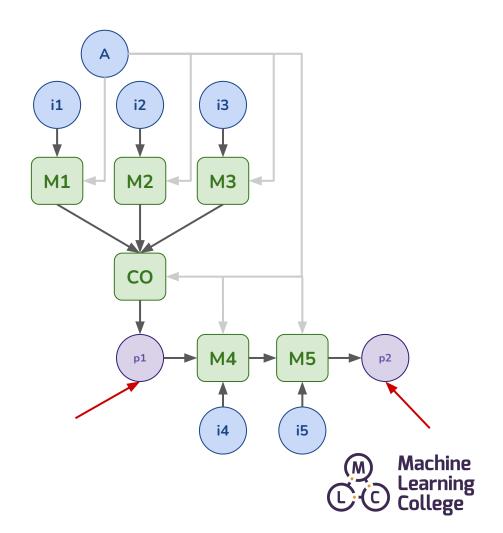
- Data preparation
 - Dataset normalization
 - Highly imbalanced dataset
- Binary classification/detection task
 - Detect starts with planets
- Model architecture
 - Dense, LSTM, Bidir. LSTM, CNN
- Training & evaluation
 - Use right evaluation metrics for imbalanced datasets



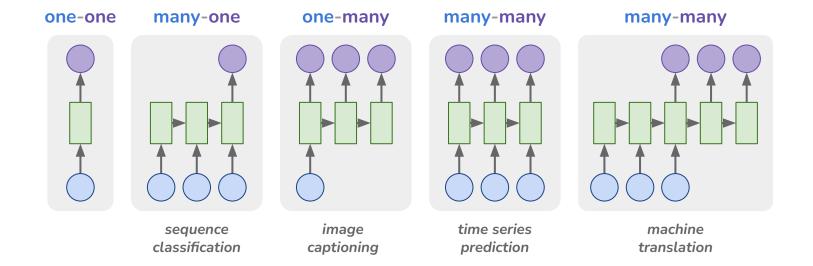


Factory process example

- Data preparation
 - Dealing with missing values
 - Dataset normalization
 - Slicing long sequences
- Regression task
 - Predict target variables in future
- Model architecture
 - Model architecture mimics the process
- Training & evaluation
 - Masking out missing labels with custom loss function

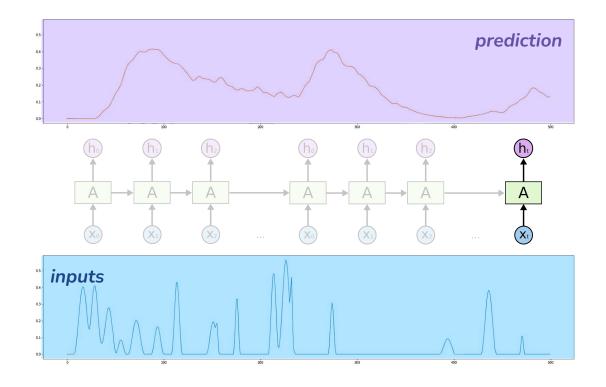


RNN and sequence data



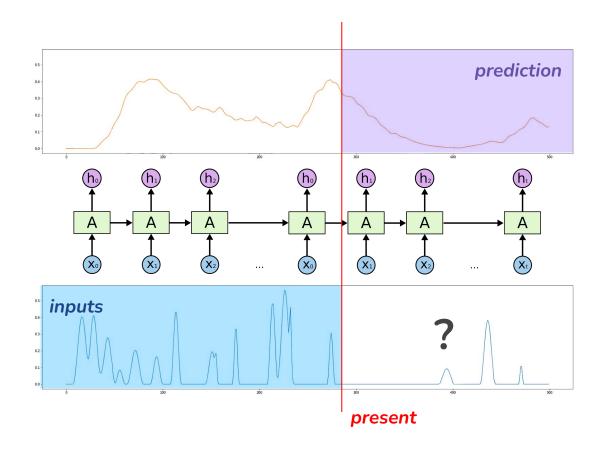


RNN for time series prediction



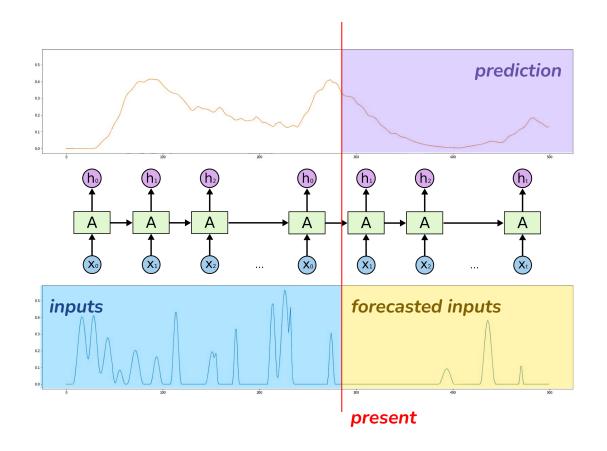


Forecasting from input variables



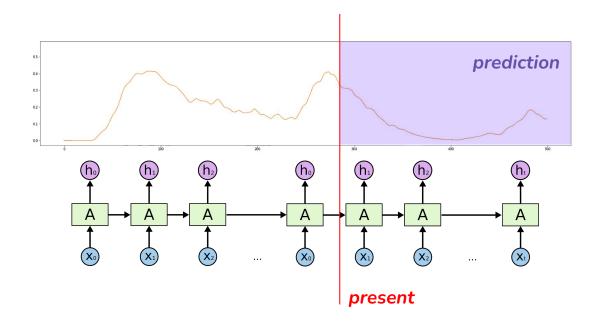


Forecasting from input variables



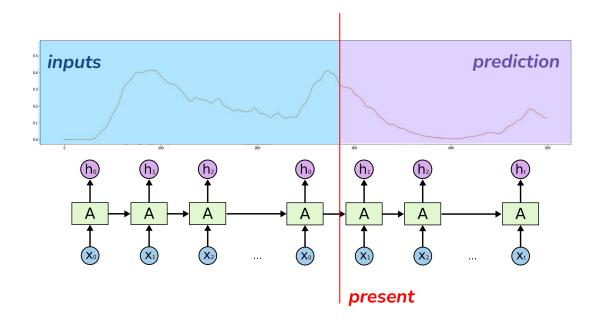


Forecasting from historical values



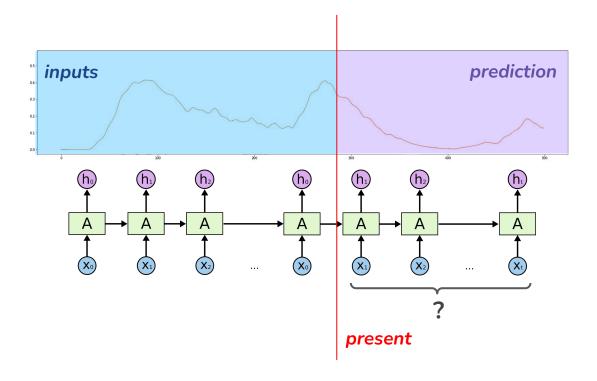


Forecasting from historical values



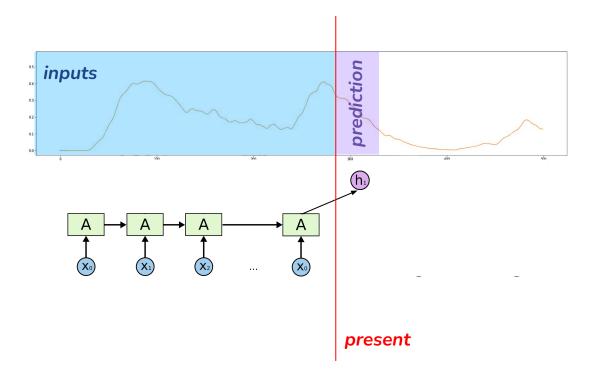


Forecasting from historical values



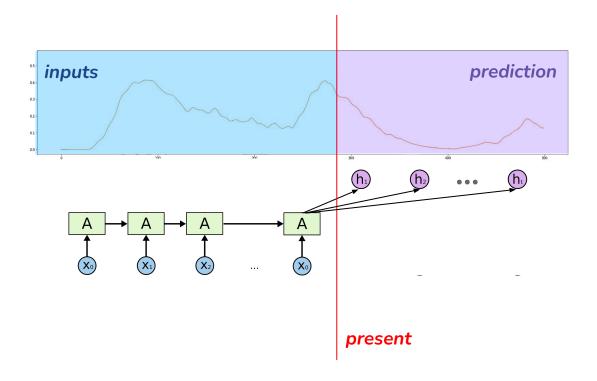


Forecasting – one step ahead



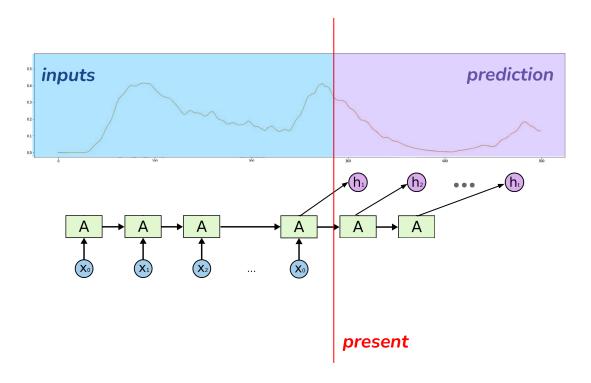


Forecasting – flat multi-step prediction



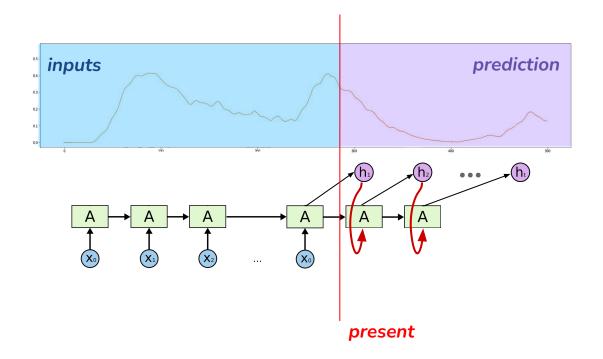


Forecasting – developed multi-step predition



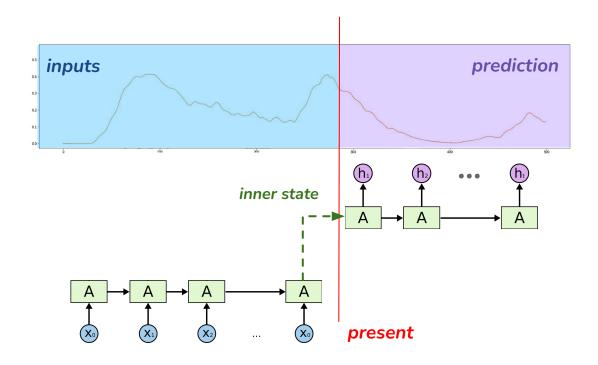


Forecasting – developed multi-step predition

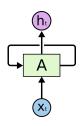


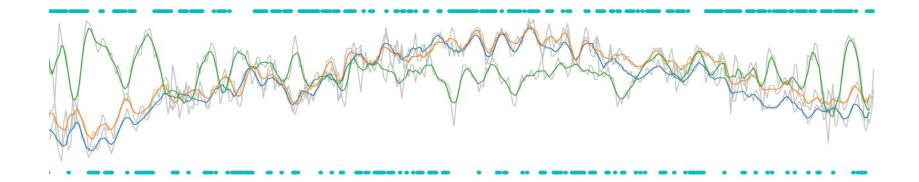


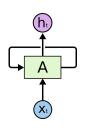
Forecasting – encoder & decoder



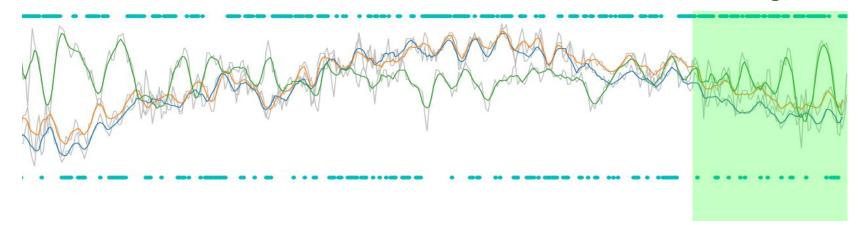


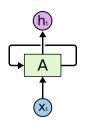




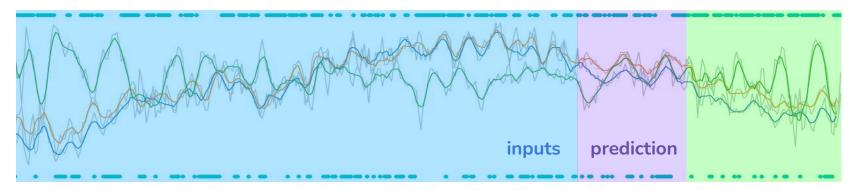


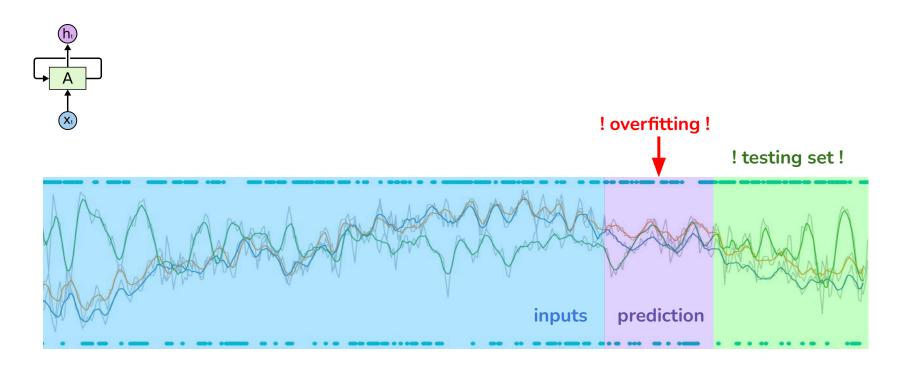
! testing set!

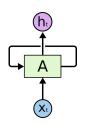




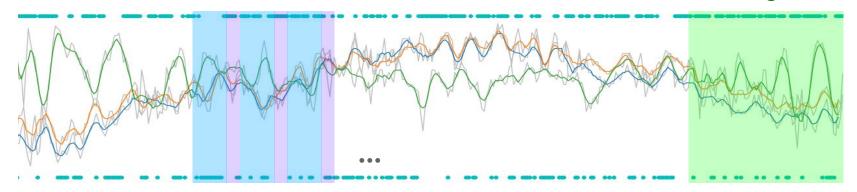
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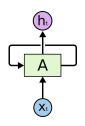




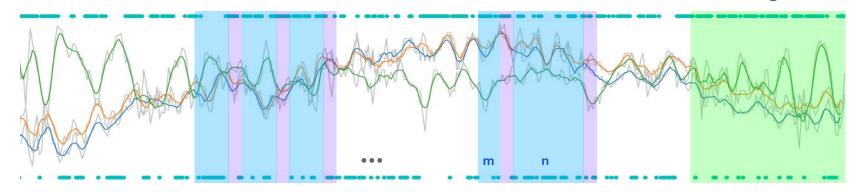


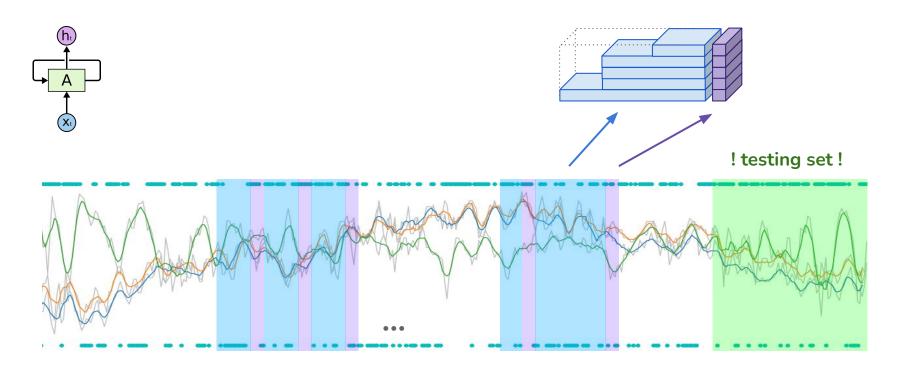
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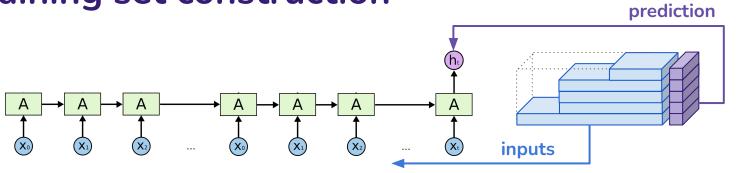




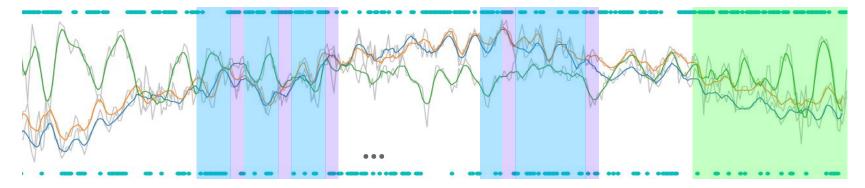
! testing set!





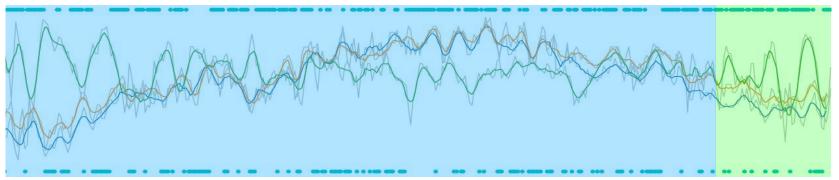


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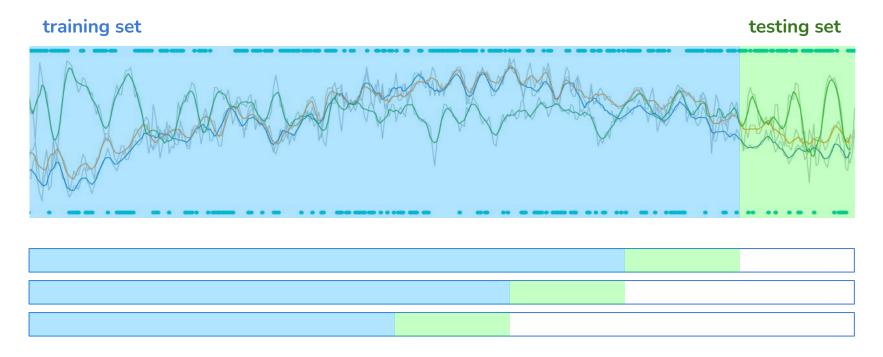


Training set construction

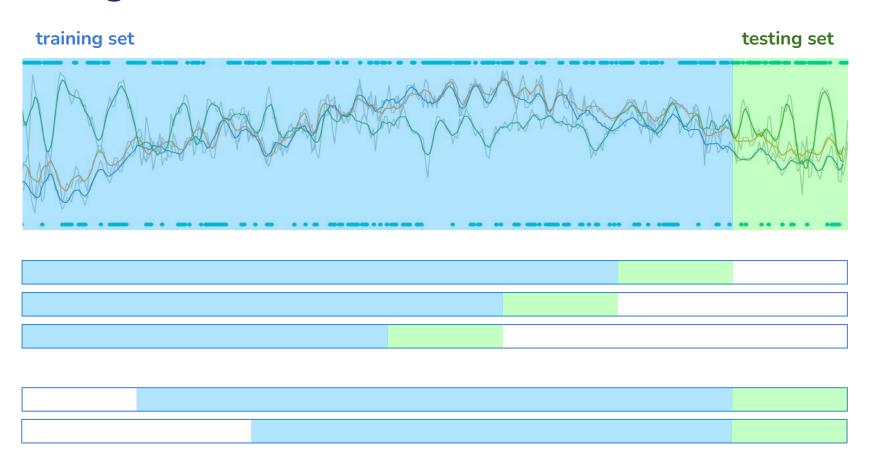




Training set construction

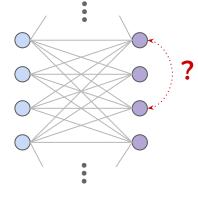


Training set construction

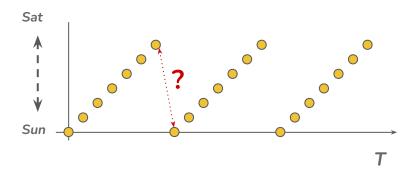


Feature Encoding – Seasonal dummy variables

0	0	0	0
1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1
0	0	0	0
0	0	0	0
	1 0 0 0	1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 0 0 0 1 0 0 0 1 0 0 0 0 0 0

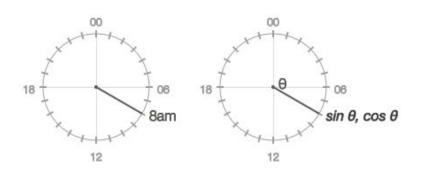


- (hour of day, day of week, ...)
- Numerical variables
- One-hot encoding

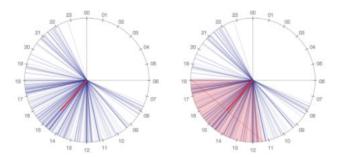


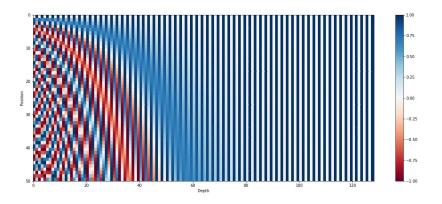
https://medium.com/life-at-hopper/ai-in-travel-part-2-representing-cyclic-and-geographic-features-4ada33dd0b22 https://kazemnejad.com/blog/transformer_architecture_positional_encoding/

Feature Encoding – Seasonal dummy variables



- Circular encoding
- Positional embedding (transformers)

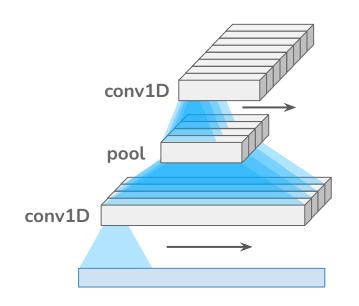


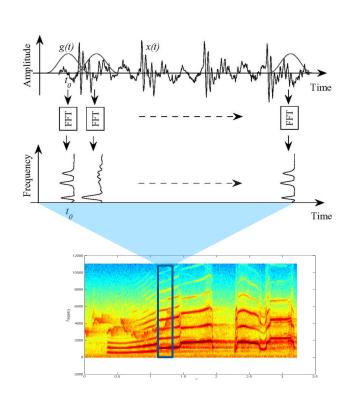


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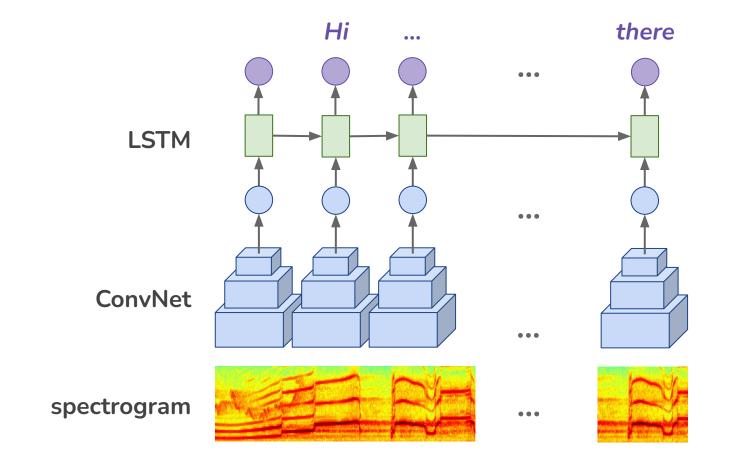
Feature Encoding II

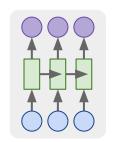
- Exchange for extra dimension
 - 1D Convolution & pooling
 - Short-Time Fourier Transform





Advanced architectures







Additional learning materials

Classical time series

- <u>Time series course</u> a book-like explanation of basic principles of time-series and classical analysis
- Statistical forecasting detailed notes on classical time series analysis and ARIMA models

Keras

- Guides code examples for most of the basics in Keras
- <u>Examples</u> huge selection of code examples from different areas (time series, vision, ...)
- Blog good selection of advanced application of Keras on practical problems

Interesting blogs

- Adam Geitgey Machine learning is fun great selection of simple examples from various areas
- Christopher Olah very well-described principles of neural networsk (with a lot of visual insights)
- Andrej Karpathy some very interesting insights (including the debug recipes for NNs)
- <u>Distill</u> Chris Olah and Shan Carter collaboration open problems in deep learning & advanced topics

Tech companies blogs

- <u>DeepMind (Google)</u> top research in artificial intelligence usually acompanied with science papers
- OpenAl started as non-commercial research group / answer to Deepmind
- Facebook many interesting projects sometimes with free-to-use pre-learned models
- Amazon many interesting machine learning articles sometimes with detailed papers



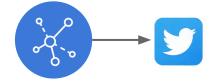
Time series prediction from textual data





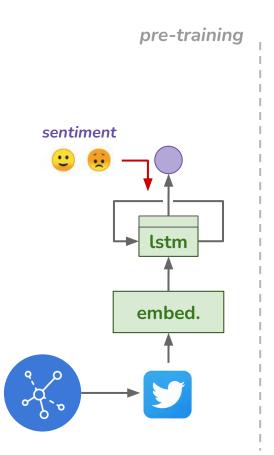
Time series prediction from textual data







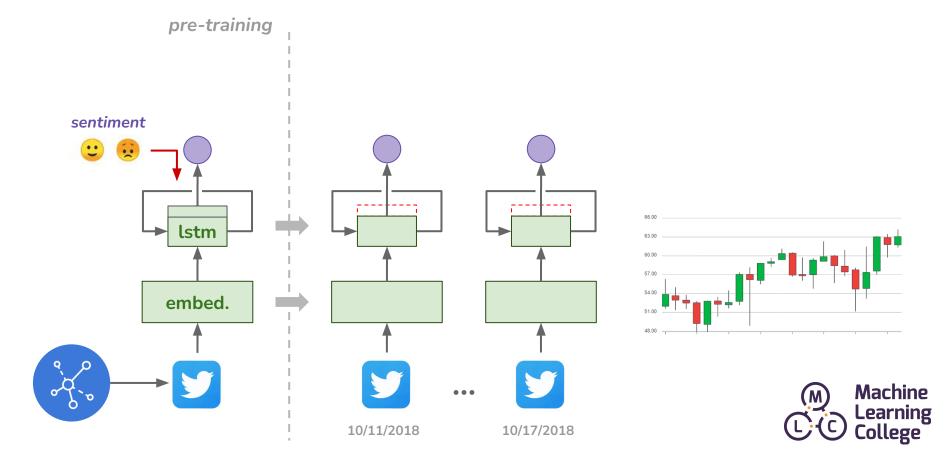
Pre-training with additional data



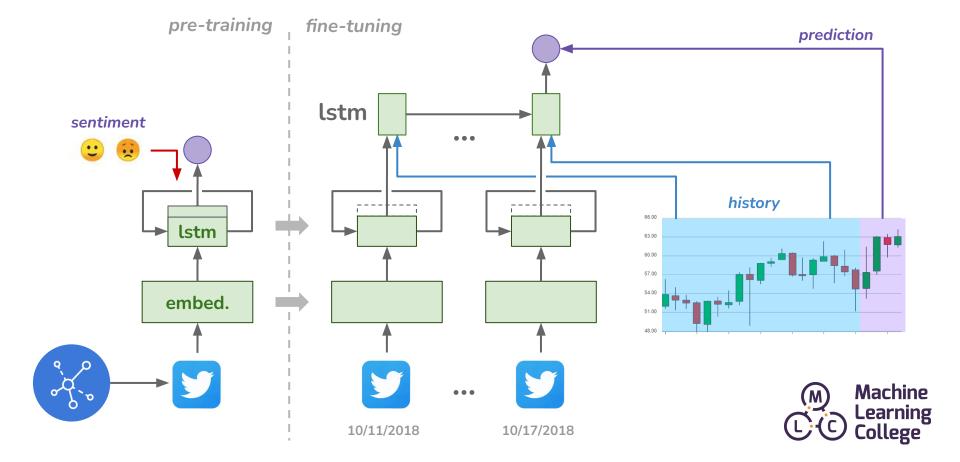




Transfering model & exposing feature layer



Fine-tuning with time series target data



Fine-tuning with time series target data

