Time Aware Machine Learning

Mark Steadman
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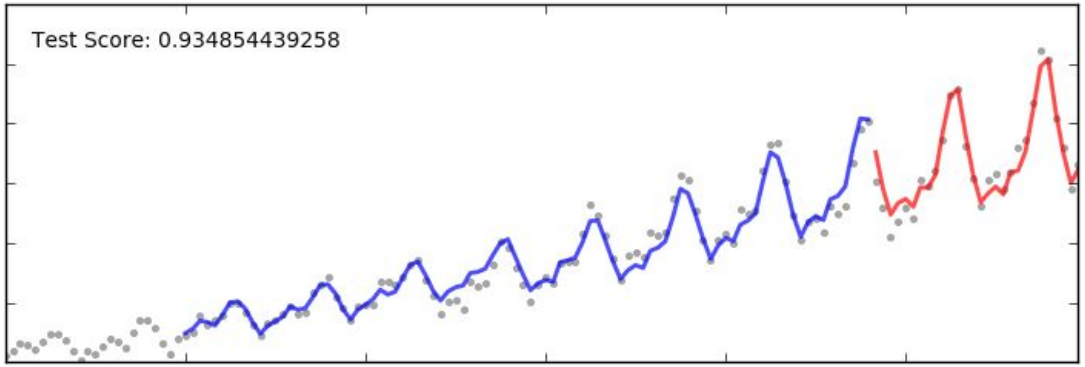
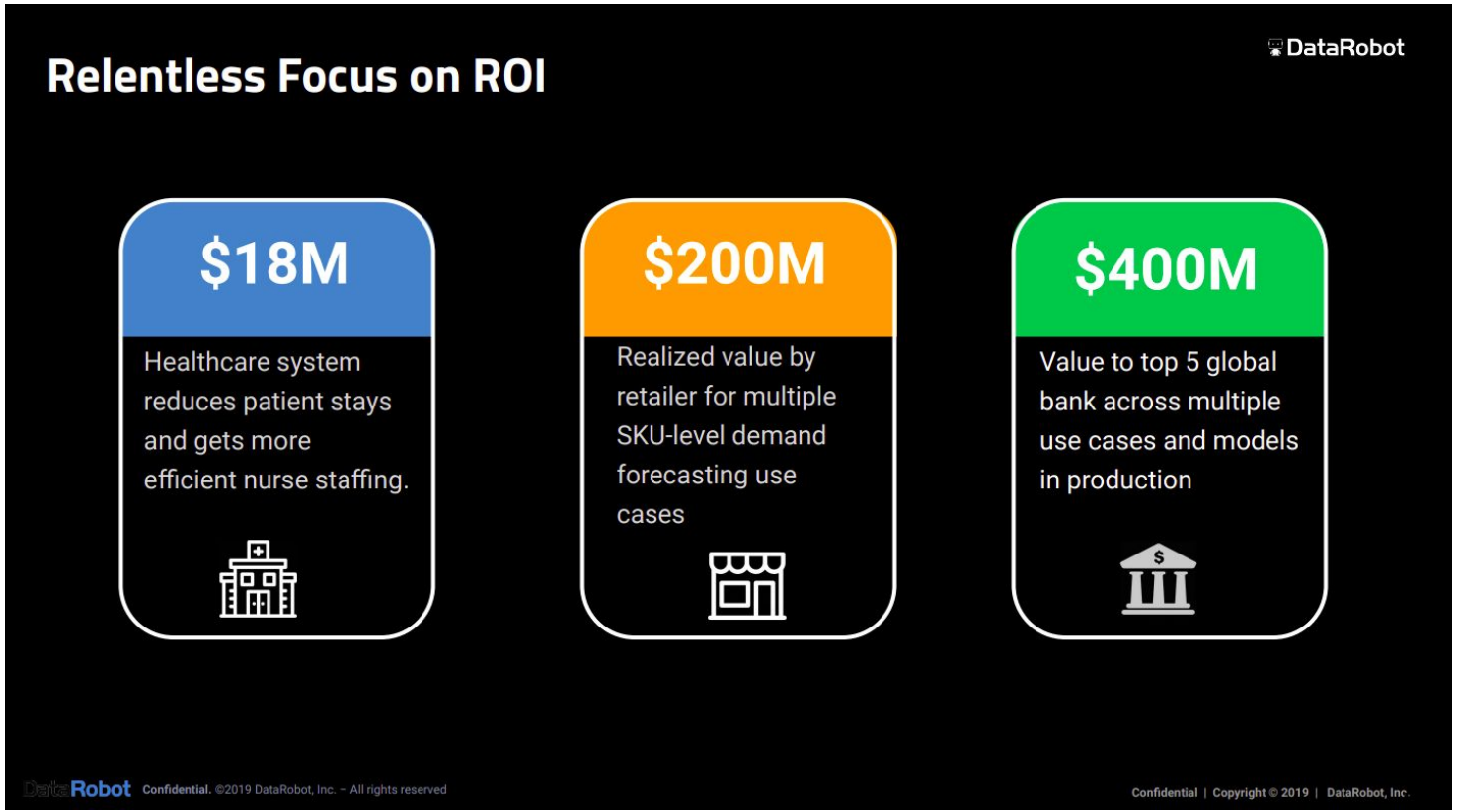


Many of the most valuable problems involve time



What is Time Aware Machine Learning?

Machine Learning Makes Some Key Assumptions

The main one that concerns us to start: the data generating process is stable

- Training / Validation sets have the same distribution if split randomly
- Training / Prediction sets have the same distribution

But this often does not hold

- Events can change the distribution
- Data can “drift” over time as the system evolves
- Data can “drift” over time as the data evolves

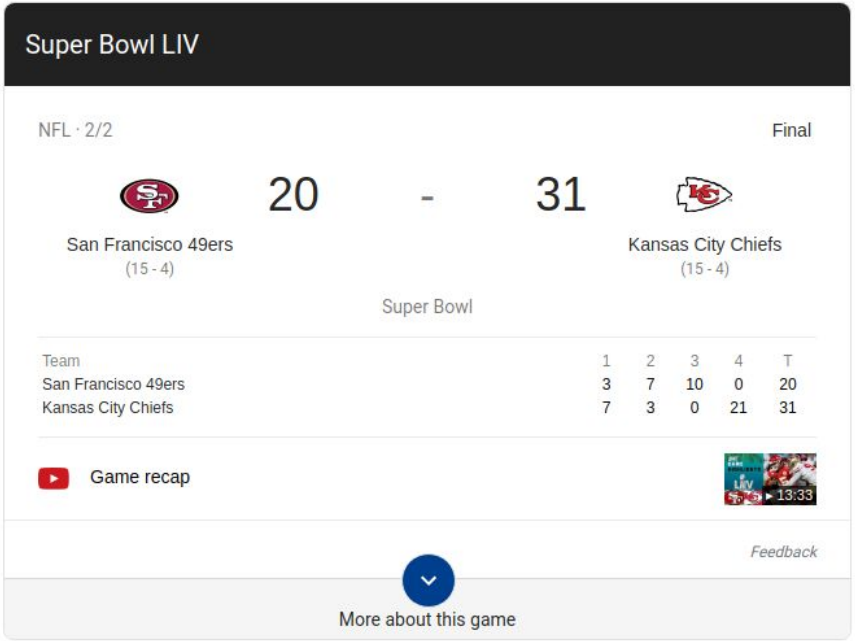
Pre-Event And Post Event Can Be Quite Different

FanDuel Sportsbook ✓
@FDSportsbook

Updated Super Bowl Odds 🏆

🏈➡️ go.fanduel.com/NFL.Futures

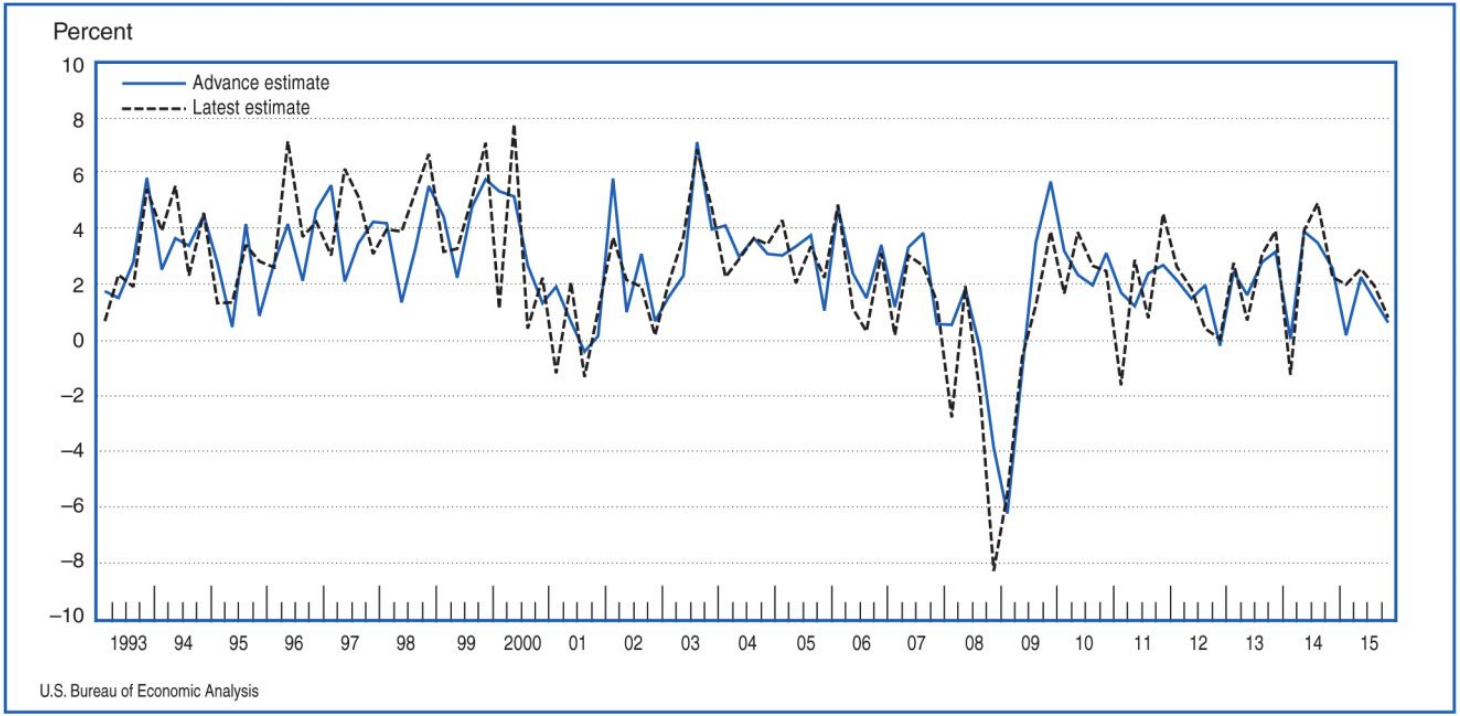
10:27 AM · Aug 26, 2019 · Twitter Web App



Your System Can Evolve Over Time

Historical Data Can Update As Well

Chart 1. Percent Change in Real Gross Domestic Product, 1993–2015



Dates and Times Pose Particular Challenges As Features

- Given “2020-04-01 23:09:12.004256” how to put it into your model?
  - Need to encode somehow
- They can cause overfitting even if encoded as they often behave like IDs
  - Knowing that any email that arrives at 2020-04-01 23:09:12.004256 is spam is often not helpful and doesn’t generalize
- There are a host of other consistency challenges
  - Daylight savings time?
  - What date is 04/01/2020?

What is Time-Aware Machine Learning (TAML)

It is about performing ML in the following situations

- Date or time variables are important to the overall context of the problem
- You want to use date or time variables in your models

Agenda

- Introduction to time series modeling
- Approach 1: Machine Learning + Feature Engineering
- Exercise
- Approach 2: Deep Learning
- Group exercise

Time Series Exercise

Prerequisites

- Python 3.6+ / 2.7 Jupyter Notebook
- numpy>=1.16, pandas>=0.24,
  scikit-learn>=0.20, matplotlib, IPython

Instructions

https://github.com/vikua/time-series-workshop

What is a Time Series?

Predict future values based on past and present data

Sales... Search Sheet

Home Insert Page Layout Formulas Data Review Share

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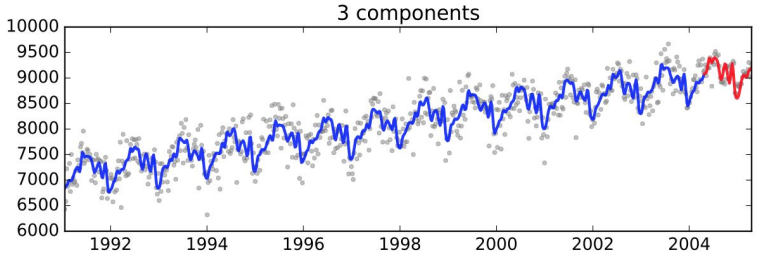
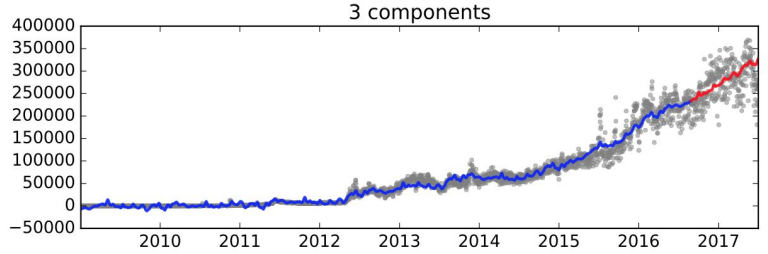
	A	B	C	D	E	F	G
1	Week	Sales	Online_Ad_Spend	TV_Ad_Spend	Flyer_Spend	Web_Total_Visits	Web_Unique_Visitors
2	1/6/2013	122759290	459742	208609.59	139779.87	392489	60865
3	1/13/2013	122837816.9	455624.07	636317.34	108928.9	481396	74594
4	1/20/2013	122330234.3	306977.25	459119.52	107133.97	386720	62103
5	1/27/2013	106094594.8	222976.63	332685.78	102834.1	372462	57290
6	2/3/2013	122340940.2	393393.04	252719.83	116269.11	495301	73945
7	2/10/2013	130370810	405611.95	586970.65	102298.72	533990	76712
8	2/17/2013	120857254.2	273239.64	474100.01	124366.22	362208	56680
9	2/24/2013	123750229.4	465004.55	619069.52	111549.13	464649	69542
10	3/3/2013	119568379.1	446871.76	203441.61	125994.14	329999	53807
11	3/10/2013	129829219.8	383115.15	187667.57	106747.38	436931	62968
12	3/17/2013	122635050.3	485634.16	688591.96	102836.61	571140	82315
13	3/24/2013	130689274.2	386893.47	360485.8	105834.99	377121	54637

Sales (1) +

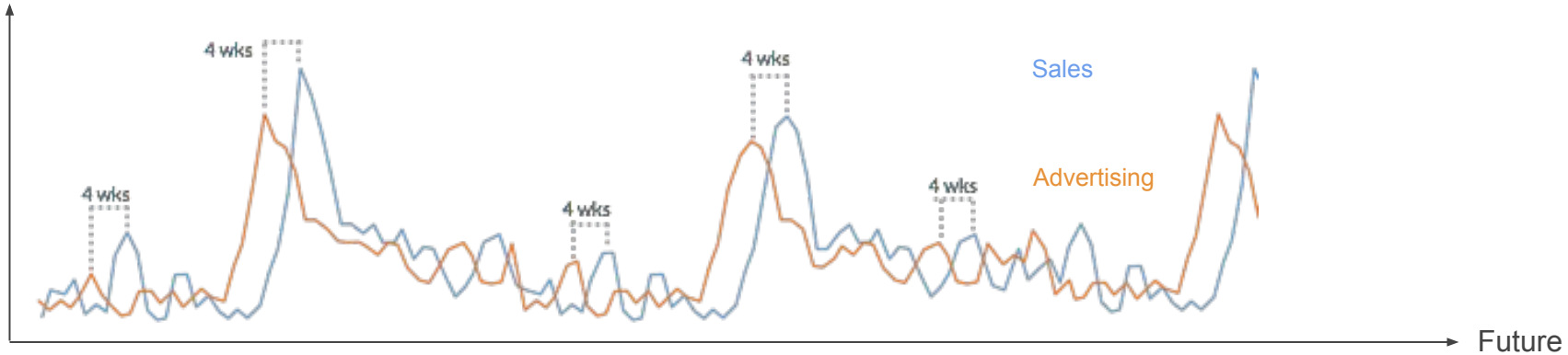
Ready 100%





Sequences as opposed to individual event data in time

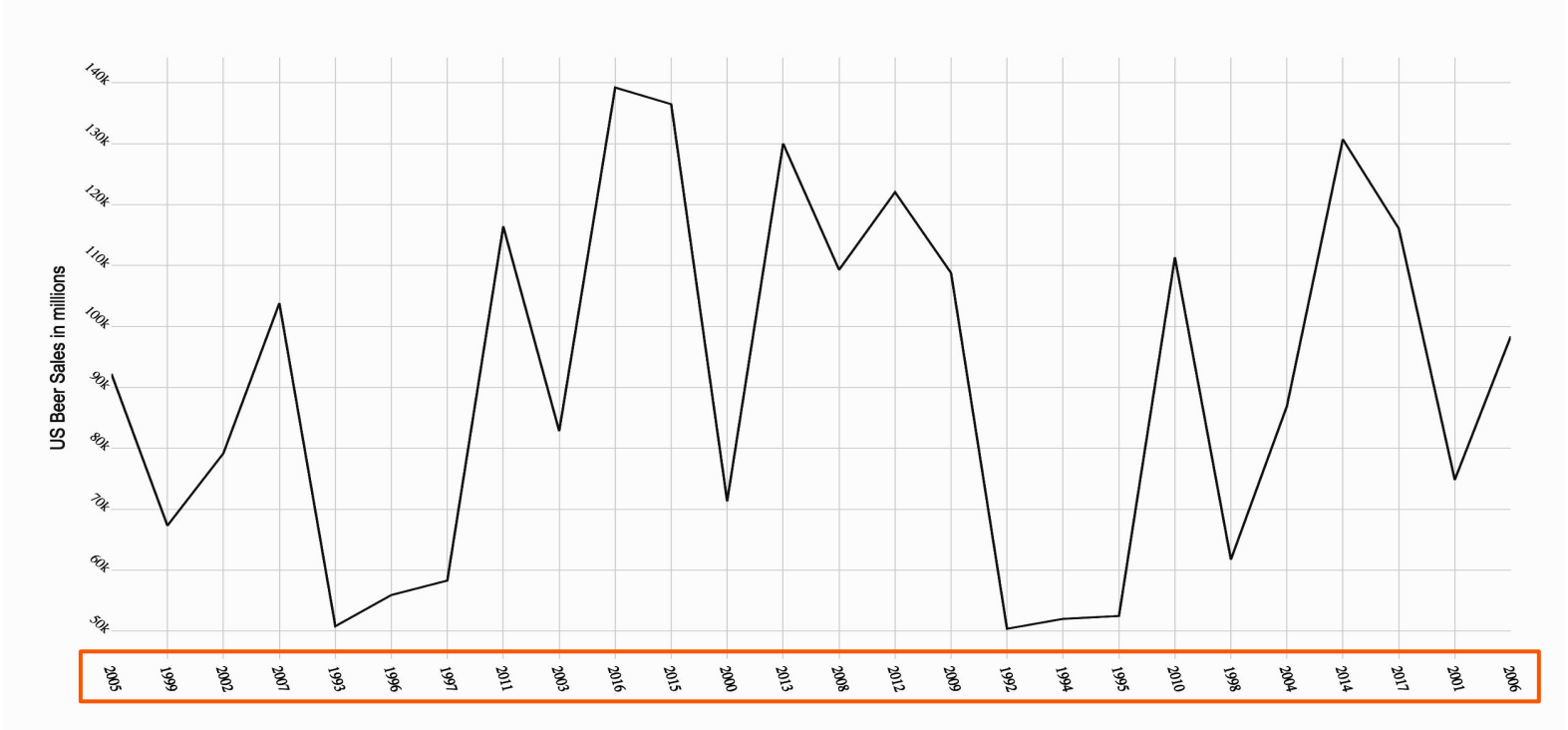
Time Series Challenges



- Real data has delays (feature engineering required)
- Difficult to validate for future predictions
- Many different treatments (stationarity, log-transform, periodic)
- Many different algorithms (ARIMA, Exp Smoothing, Decompositions)
- Most machine learning algorithms (xgboost) today are not time-aware on their own

Why are Time Series Problems Different? US Beer Sales

Common assumption #1: Order of rows doesn't matter



Why are Time Series Problems Different? US Beer Sales

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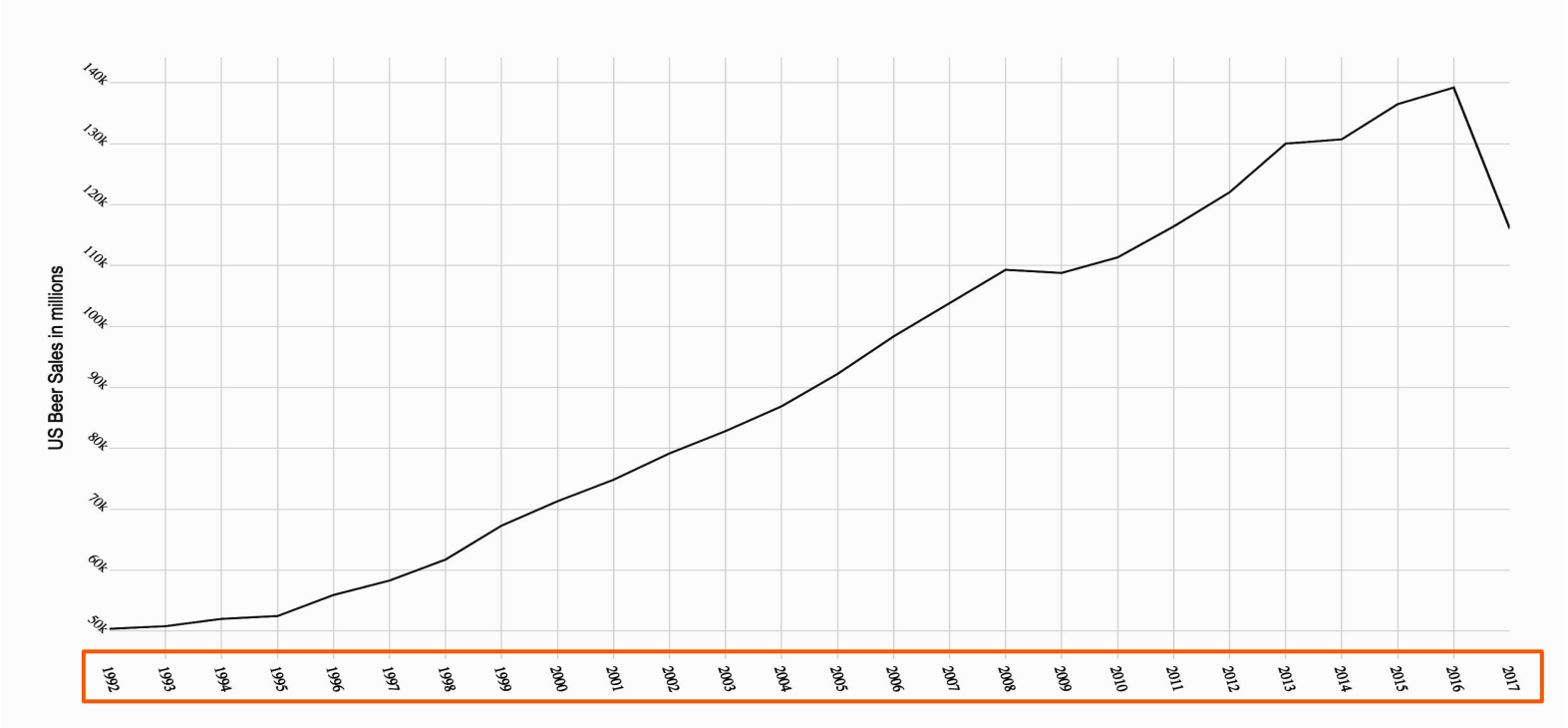
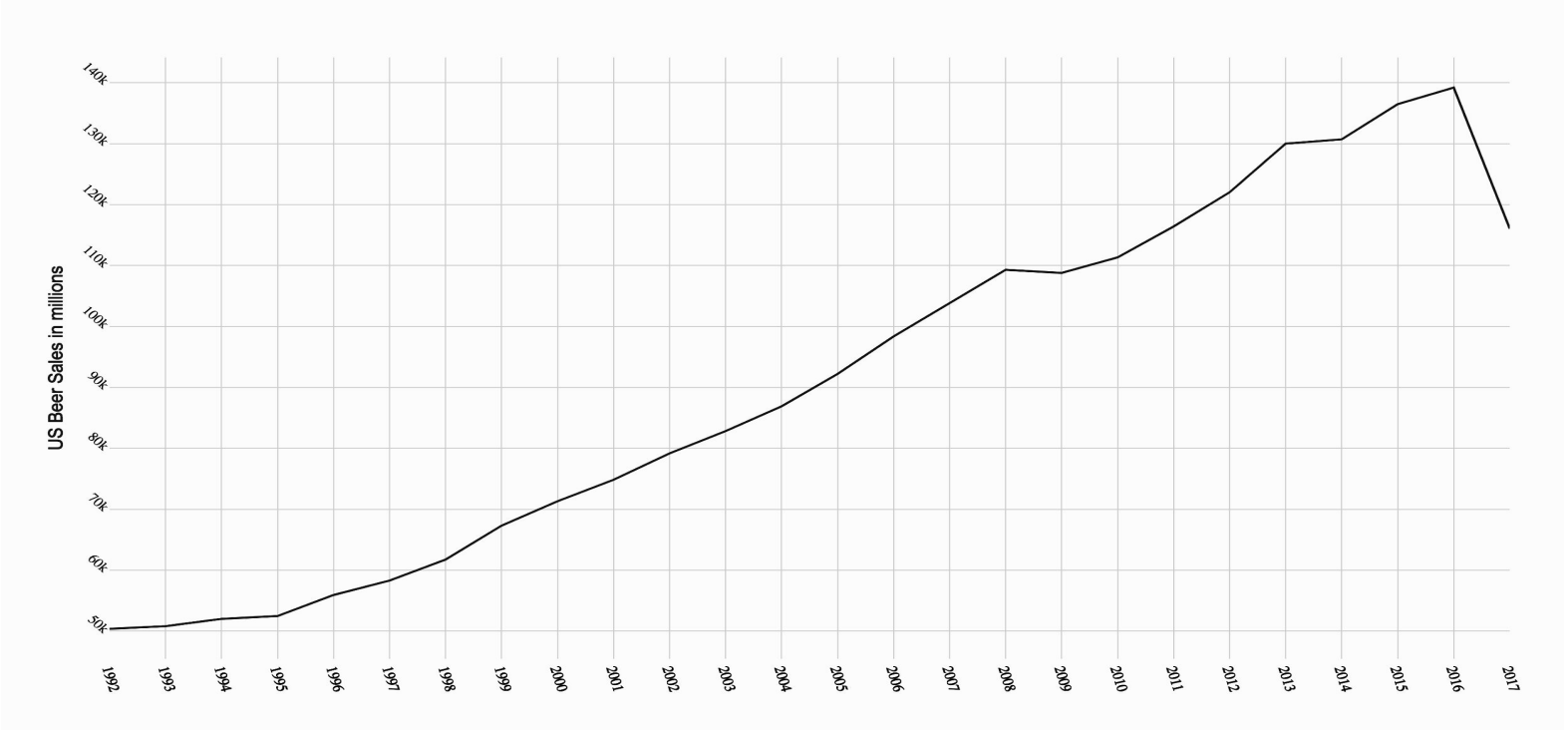


Why are Time Series Problems Different? US Beer Sales

Common assumption #2: Training and future data are similar



Why are Time Series Problems Different? US Beer Sales

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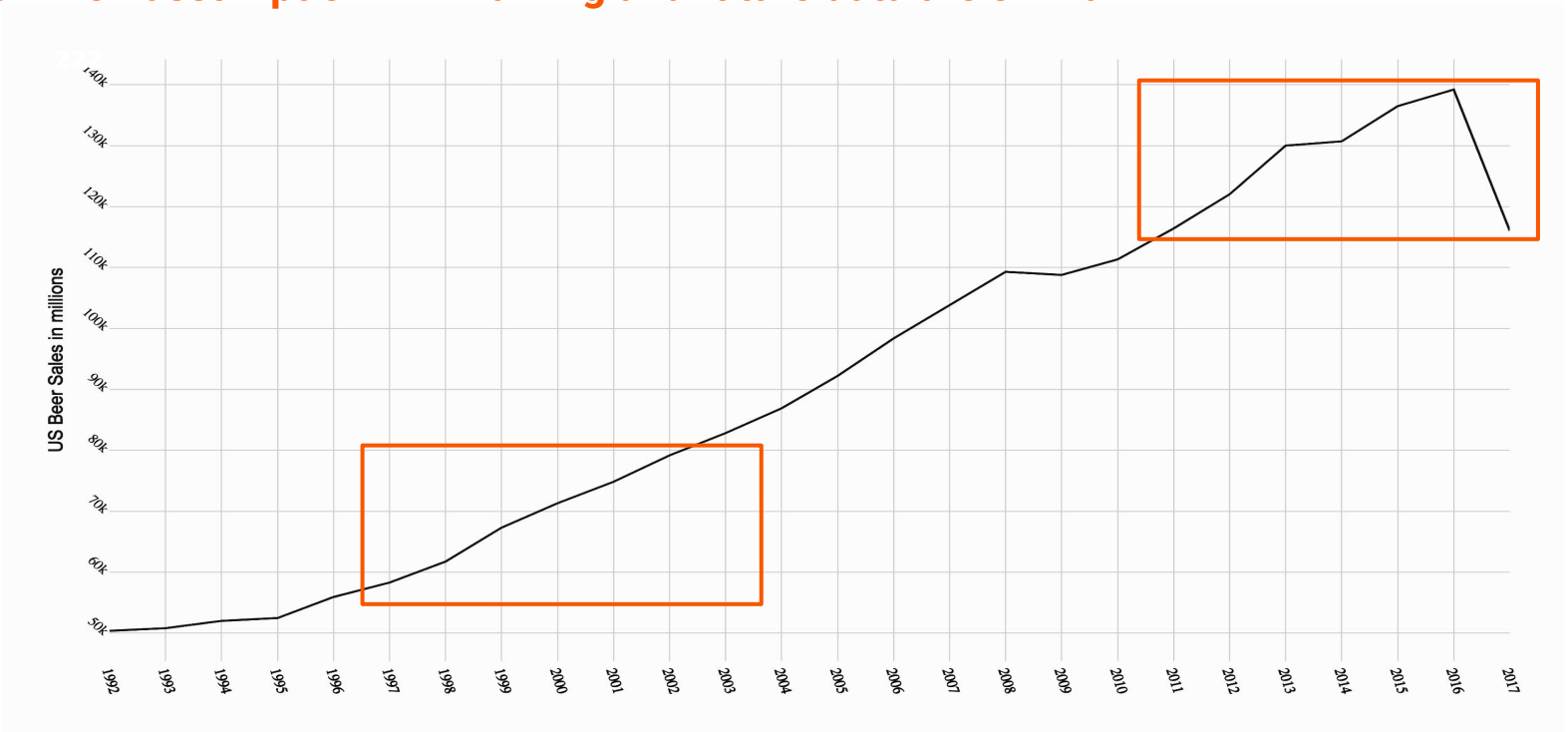

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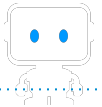
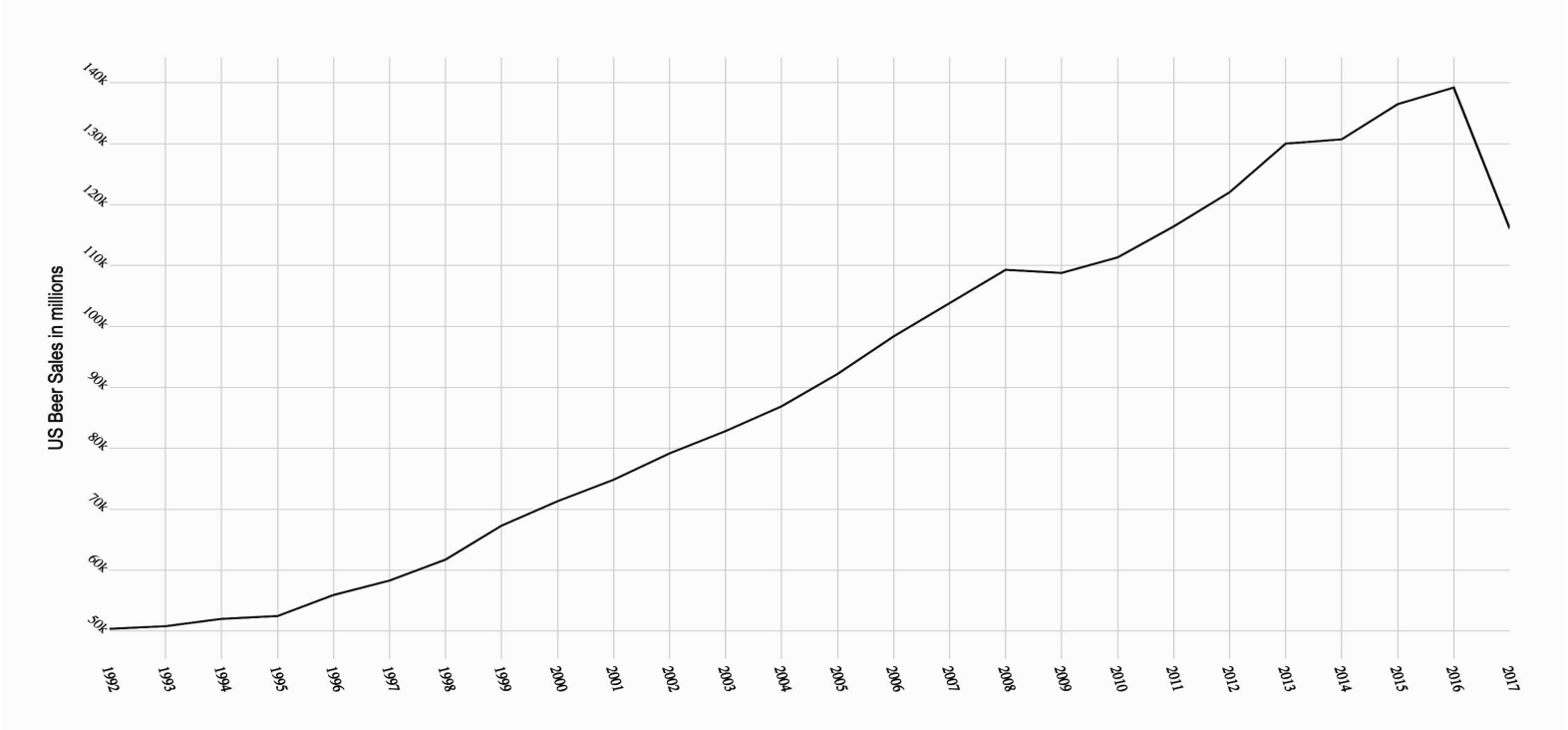


Common assumption #3: Models can be evaluated with a single row of data



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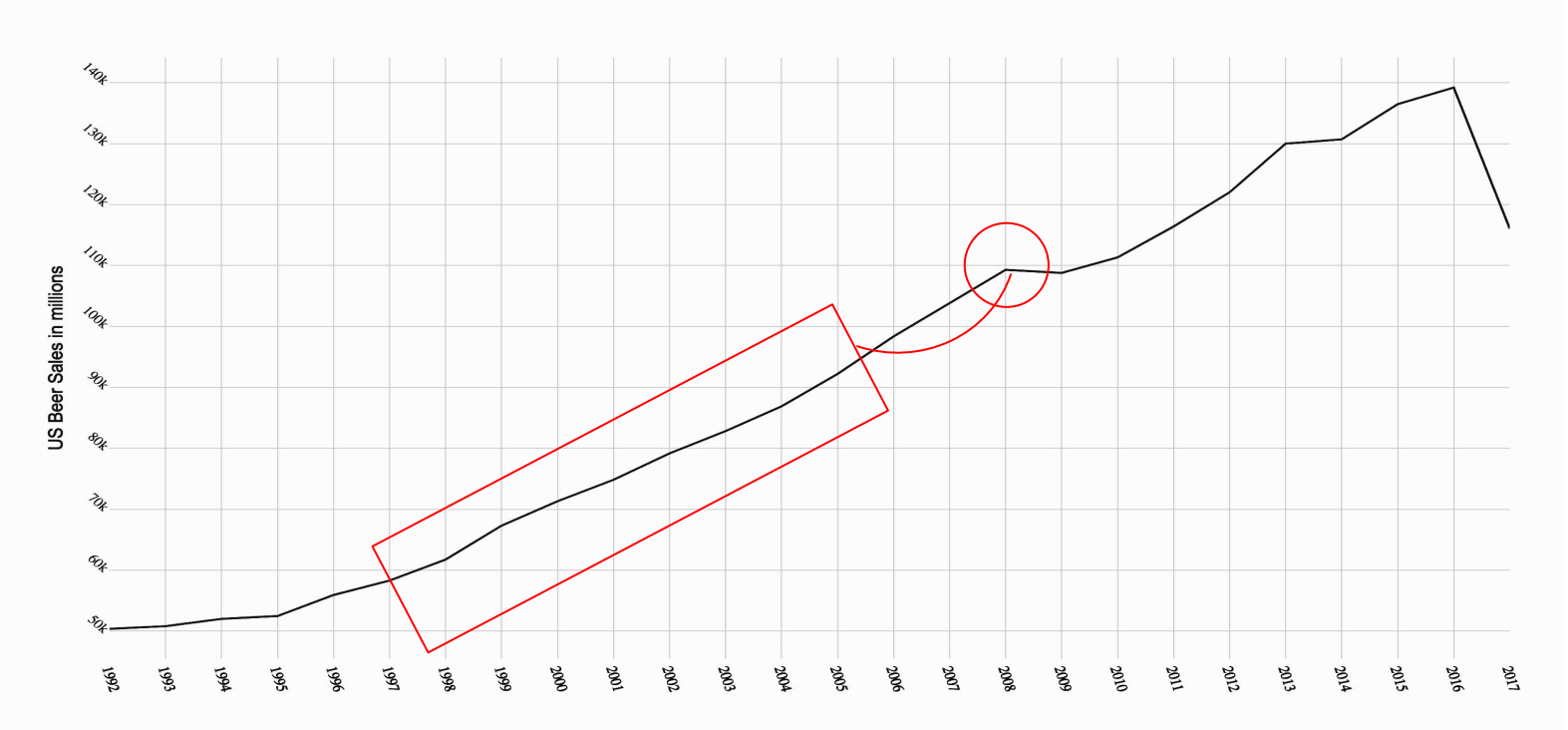


Time Series Machine Learning

Feature Engineering

- Automated lag selection
- Automated window statistics
- Rolling numeric, categorical, text information

Target Transforms

- Stationarity, exponential, periodicity detection
- Automated differencing, offsets, link functions, log transformations
- Additive or multiplicative models

Model Backtesting

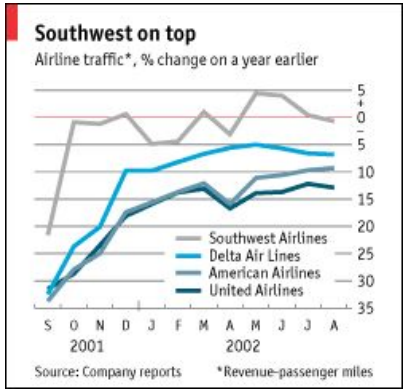
- Time-aware data partitioning and validation
- Automated or configurable backtesting strategies
- Refit on most recent data

Modeling

- Classical time series models (ARIMA, ETS, decompositions)
- Time-aware xgboost, distance modeling, and other algorithms
- Deploy to dedicated prediction service

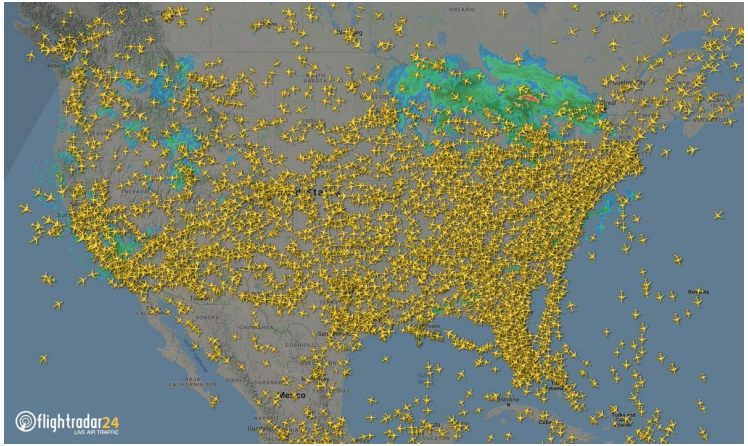
Types of Time Series Problems

Strategic



- Few series
- Traditional approaches often due well
- Sufficient History
- Longer refresh periods

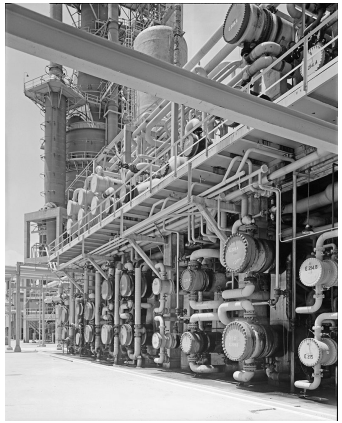
Operational



- Many series
- Insufficient history → routes start and stop
- Shorter refresh periods → need a forecast every day

Two Types of Complexity in Machine Learning

The Refinery



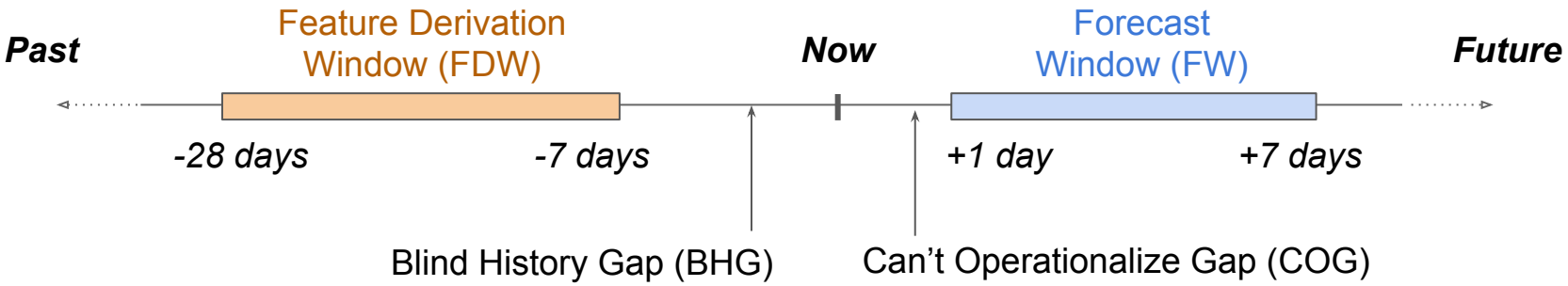
- Complexity is in the pipeline
- Each step is understandable but how to put them together?
- Parallelizable but infrastructure heavy

The Plan

$$
\begin{aligned}
&\delta\mu + \left[(\mu+p)\,v^{\alpha} + (\delta\mu+\delta p)\,v^{\alpha} + \Pi^{\alpha}_{\beta}v^{\beta}\right]v_{\alpha} - 2\,(\mu+p)\,C_{\alpha\beta}v^{\alpha}v^{\beta} \\
&\qquad = \sum_{J}\Big\{\delta\mu_{(J)} + \left[\left(\mu_{(J)}+p_{(J)}\right)v^{\alpha}_{(J)} + \left(\delta\mu_{(J)}+\delta p_{(J)}\right)v^{\alpha}_{(J)} + \Pi_{(J)\beta}^{\alpha}v^{\beta}_{(J)}\right]v_{(J)\alpha} \\
&\qquad\quad - 2\left(\mu_{(J)}+p_{(J)}\right)C_{\alpha\beta}v^{\alpha}_{(J)}v^{\beta}_{(J)}\Big\}, \\
&\delta p + \tfrac{1}{3}\left[(\mu+p)\,v^{\alpha} + (\delta\mu+\delta p)\,v^{\alpha} + \Pi^{\alpha}_{\beta}v^{\beta}\right]v_{\alpha} - \tfrac{2}{3}\,(\mu+p)\,C_{\alpha\beta}v^{\alpha}v^{\beta} \\
&\qquad = \sum_{J}\Big\{\delta p_{(J)} + \tfrac{1}{3}\left[\left(\mu_{(J)}+p_{(J)}\right)v^{\alpha}_{(J)} + \left(\delta\mu_{(J)}+\delta p_{(J)}\right)v^{\alpha}_{(J)} + \Pi_{(J)\beta}^{\alpha}v^{\beta}_{(J)}\right]v_{(J)\alpha} \\
&\qquad\quad - \tfrac{2}{3}\left(\mu_{(J)}+p_{(J)}\right)C_{\alpha\beta}v^{\alpha}_{(J)}v^{\beta}_{(J)}\Big\}, \\
&(\mu+p)\,v_{\alpha} + \left[\delta\mu+\delta p + \tfrac{4}{3}\,(\mu+p)\,v^{\beta}v_{\beta}\right]v_{\alpha} + \left[\Pi^{\beta}_{\alpha} + (\mu+p)\left(v_{\alpha}v^{\beta} - \tfrac{1}{3}\delta^{\beta}_{\alpha}v^{\gamma}v_{\gamma}\right)\right]v_{\beta} \\
&\qquad - \tfrac{3}{2}\,(\mu+p)\,v_{\alpha}v^{\beta}v_{\beta} - 2\Pi_{\alpha\beta}C^{\beta\gamma}v_{\gamma} = \sum_{J}\Big\{\left(\mu_{(J)}+p_{(J)}\right)v_{(J)\alpha} \\
&\qquad + \left[\delta\mu_{(J)} + \delta p_{(J)} + \tfrac{4}{3}\left(\mu_{(J)}+p_{(J)}\right)v^{\beta}_{(J)}v_{(J)\beta}\right]v_{(J)\alpha} \\
&\qquad + \left[\Pi_{(J)\alpha}^{\beta} + \left(\mu_{(J)}+p_{(J)}\right)\left(v_{(J)\alpha}v^{\beta}_{(J)} - \tfrac{1}{3}\delta^{\beta}_{\alpha}v^{\gamma}_{(J)}v_{(J)\gamma}\right)\right]v_{(J)\beta} \\
&\qquad - \tfrac{3}{2}\left(\mu_{(J)}+p_{(J)}\right)v_{(J)\alpha}v^{\beta}_{(J)}v_{(J)\beta} - 2\Pi_{(J)\alpha\beta}C^{\beta\gamma}v_{(J)\gamma}\Big\}, \\
&\Pi^{\alpha}_{\beta} + \left[(\mu+p)\,v^{\alpha} + (\delta\mu+\delta p)\,v^{\alpha} + \Pi^{\alpha}_{\gamma}v^{\gamma}\right]v_{\beta} - \tfrac{2}{3}\,(\mu+p)\,C^{\alpha}_{\beta}v^{\gamma}v_{\gamma} - \Pi^{\alpha\gamma}v_{\beta}v_{\gamma} \\
&\qquad - \tfrac{1}{3}\delta^{\alpha}_{\beta}\left\{\left[(\mu+p)\,v^{\gamma} + (\delta\mu+\delta p)\,v^{\gamma} + \Pi^{\gamma}_{\delta}v^{\delta}\right]v_{\gamma} - 2\,(\mu+p)\,C_{\gamma\delta}v^{\gamma}v^{\delta}\right\} \\
&\qquad = \sum_{J}\Big\{\Pi_{(J)\beta}^{\alpha} + \left[\left(\mu_{(J)}+p_{(J)}\right)v^{\alpha}_{(J)} + \left(\delta\mu_{(J)}+\delta p_{(J)}\right)v^{\alpha}_{(J)} + \Pi_{(J)\gamma}^{\alpha}v^{\gamma}_{(J)}\right]v_{(J)\beta} \\
&\qquad\quad - \tfrac{2}{3}\left(\mu_{(J)}+p_{(J)}\right)C^{\alpha}_{\beta}v^{\gamma}_{(J)}v_{(J)\gamma} - \Pi^{\alpha\gamma}_{(J)}v_{(J)\beta}v_{(J)\gamma} - \tfrac{1}{3}\delta^{\alpha}_{\beta}\Big\{\left[\left(\mu_{(J)}+p_{(J)}\right)v^{\gamma}_{(J)}\right. \\
&\qquad\quad \left. + \left(\delta\mu_{(J)}+\delta p_{(J)}\right)v^{\gamma}_{(J)} + \Pi_{(J)\delta}^{\gamma}v^{\delta}_{(J)}\right]v_{(J)\gamma} - 2\left(\mu_{(J)}+p_{(J)}\right)C_{\gamma\delta}v^{\gamma}_{(J)}v^{\delta}_{(J)}\Big\}\Big\}.
\end{aligned}
\tag{31}
$$

- Complexity is in the model
- How to understand and control what the model is doing?
- How to train?

General Time Series Framework



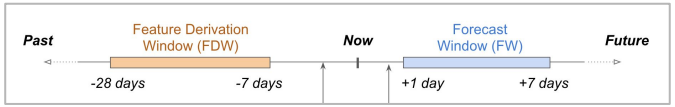
Simple Lags

	Date	Sales	Sales 3 days ago	Number of Employees	Ad Spending	Inventory Rate	Weather
	11/09/17	$432,897					
	11/10/17	$474,306					
	11/11/17	$415,434					
	11/12/17	$289,290	$432,897	16	$3,000	47%	Rain
	11/13/17	$355,786	$474,306	19	$2,100	46%	Heavy Wind
today	11/14/17	$375,284	$415,434	17	$1,200	41%	Cloudy
	...	...		...	...	...	...
tomorrow	11/15/17	?	$289,290	20	$1,800	31%	Cloudy

Candidate Time Series Features

Time	Sales	Employees	Weather
1/1/17	$4,438,925	16	Rain
1/2/17	$4,703,801	17	Heavy Winds
1/3/17	$4,646,682	17	Heavy Winds
1/4/17	$4,162,316	16	Partly Cloudy
1/5/17	$2,811,162	16	Partly Cloudy
1/6/17	$3,394,591	16	Frost
1/7/17	$3,328,435	15	Heavy Winds
1/8/17	$4,227,790	15	Frost
1/9/17	$5,426,552	16	Heavy Winds
1/10/17	$4,472,594	16	Frost

+2 days



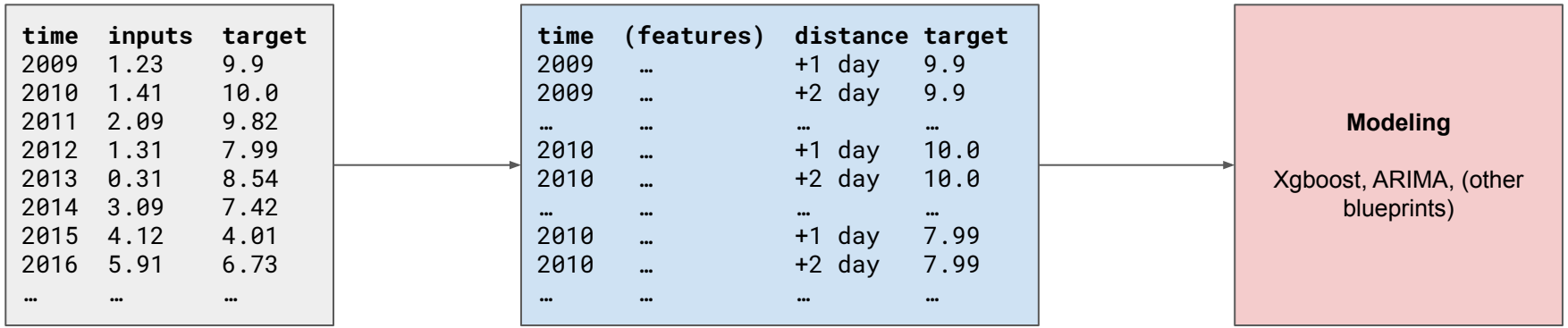
Window Features

- Rolling min, max, mean
- Rolling majority
- Rolling entropy
- Rolling text statistics
- Bollinger bands

Target Feature

- +1 day ahead
- +2 days ahead
- etc.

Time Series Feature Engineering



Original
Time Series

Derived Time Series Features
and
Forecast Target

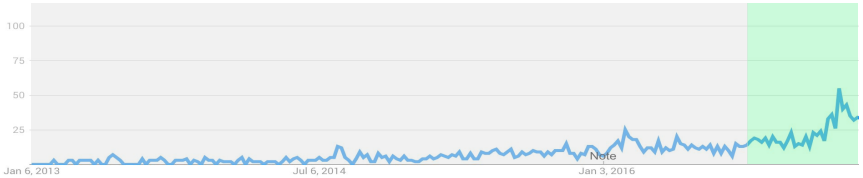
Processing and
Modeling Blueprints

Out-of-Time Validation

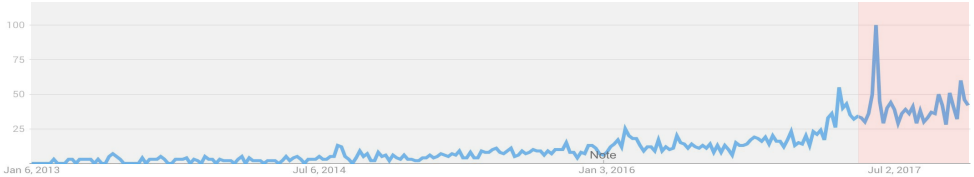
Walk-forward a set of backtests

Backtest 2

Backtest 1



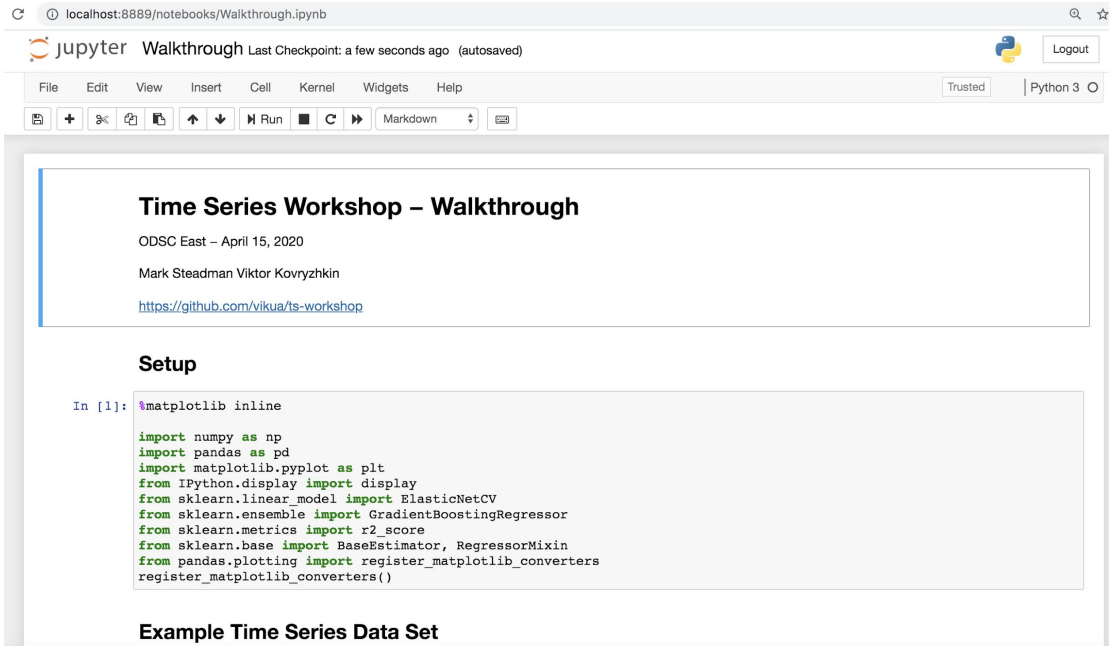
Holdout



(Total validation score) = (validation score #1) + (validation score #2) + (validation score #3) + ...

Tutorial

Walkthrough in Python



Time Series Modeling Families

Integrated Models

ARIMA, ETS, RNNs, etc.

Per Forecast Distance Models

Xgboost, elastic-net, etc.

Trends and Decomposition Models

Fourier models, linear trends, decompositions, etc.

Target Transformations

Log Transform

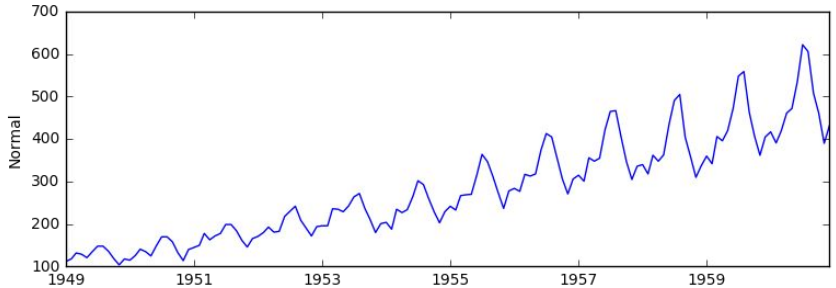
$$\log(y_t) = \log(y_{t-1}) + \log(y_{t-2}) + \ldots$$

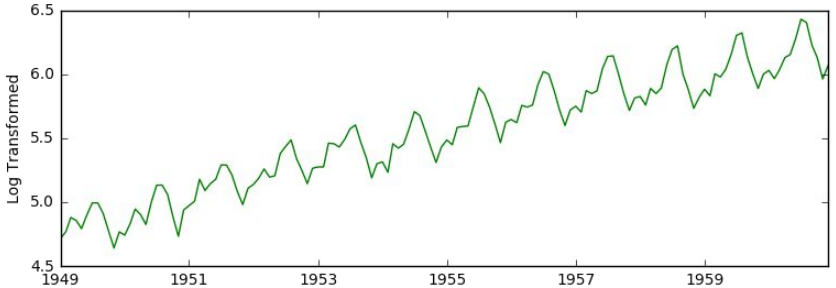
$$y_t = \exp(\log(y_{t-1}) + \log(y_{t-2}) + \ldots)$$

$$y_t = \exp(\log(y_{t-1})) * \exp(\log(y_{t-2})) * \ldots$$

$$y_t = y_{t-1} * y_{t-2} * \ldots$$

- Results in an multiplicative model (instead of additive)
- Removes exponential growth and variance



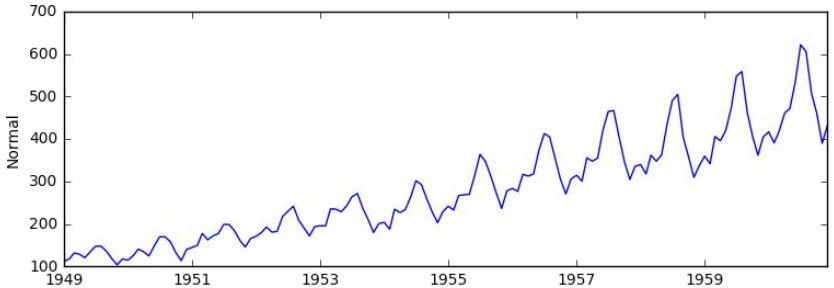


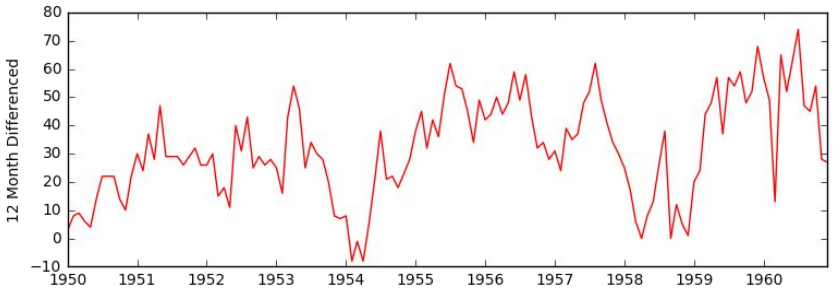
Target Transformations

Differencing

$$y_t - y_{t-p} = y_{t-1} + y_{t-2} + \ldots$$

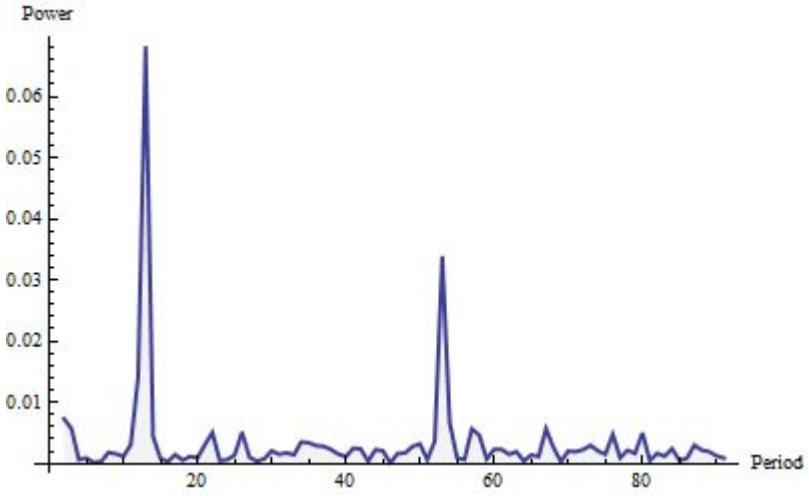
- Removes trend and periodicity / creates a more stationary signal



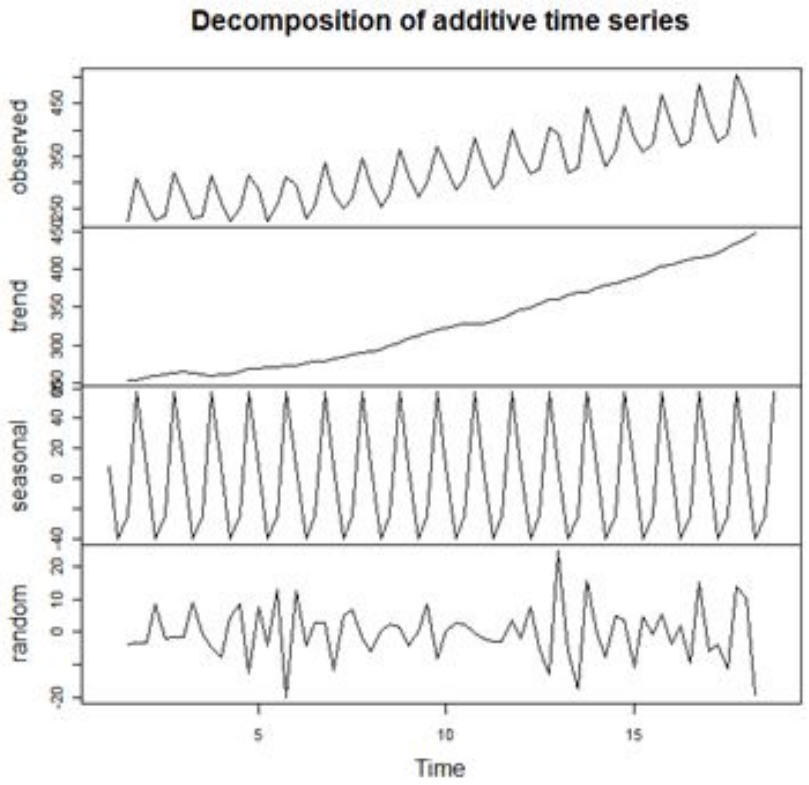


Periodicity / Periodogram

Periodic pattern detection



Time Series Decomposition



Observed data

=

Trend component

+

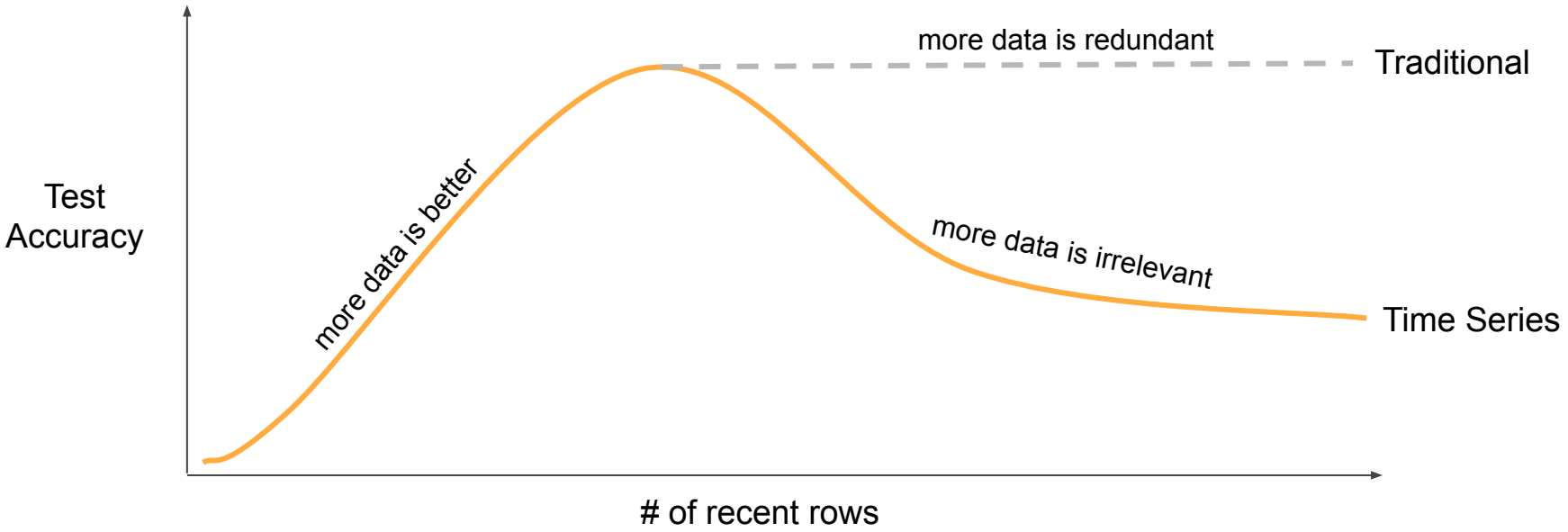
Annual seasonal component

+

Annual seasonal component

How much data

Time series learning curves

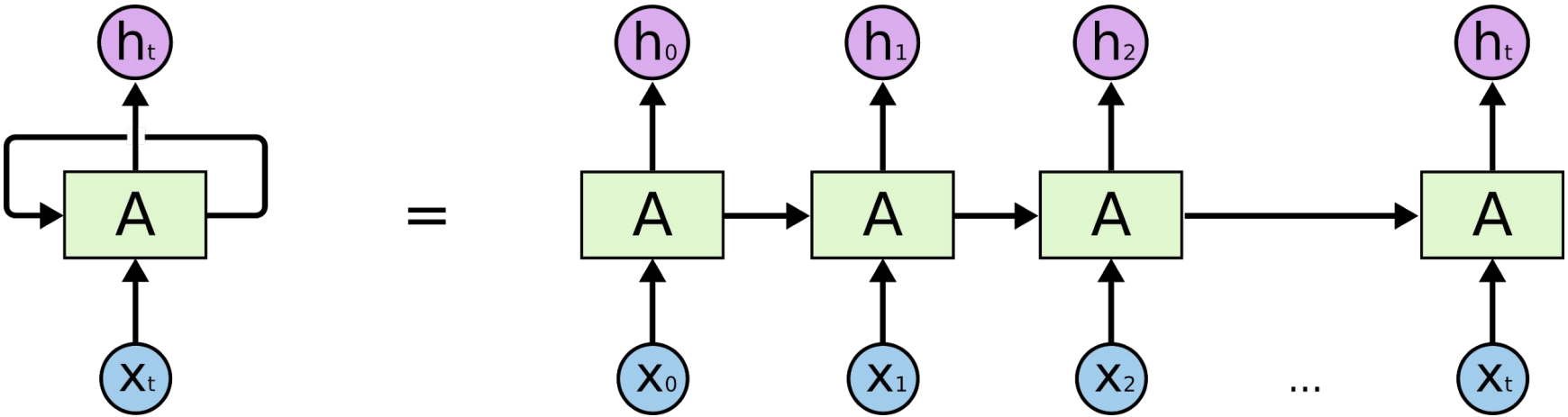


If you have a large big dataset and you train a very big neural network, then success is guaranteed!

Ilya Sutskever

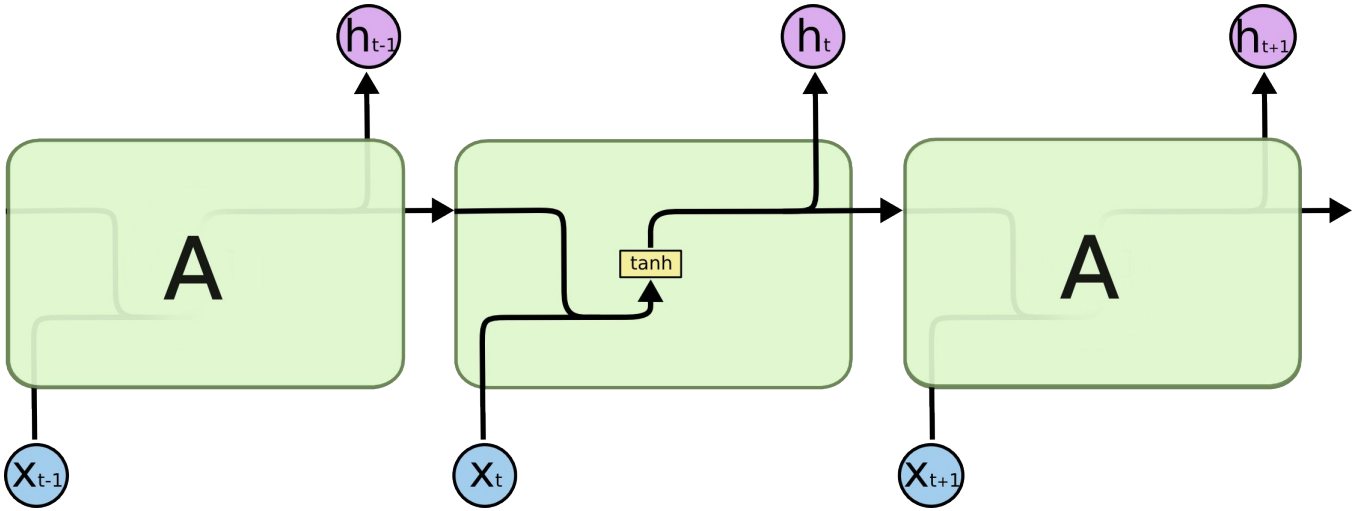
Deep learning - success is guaranteed.

RNN refresher



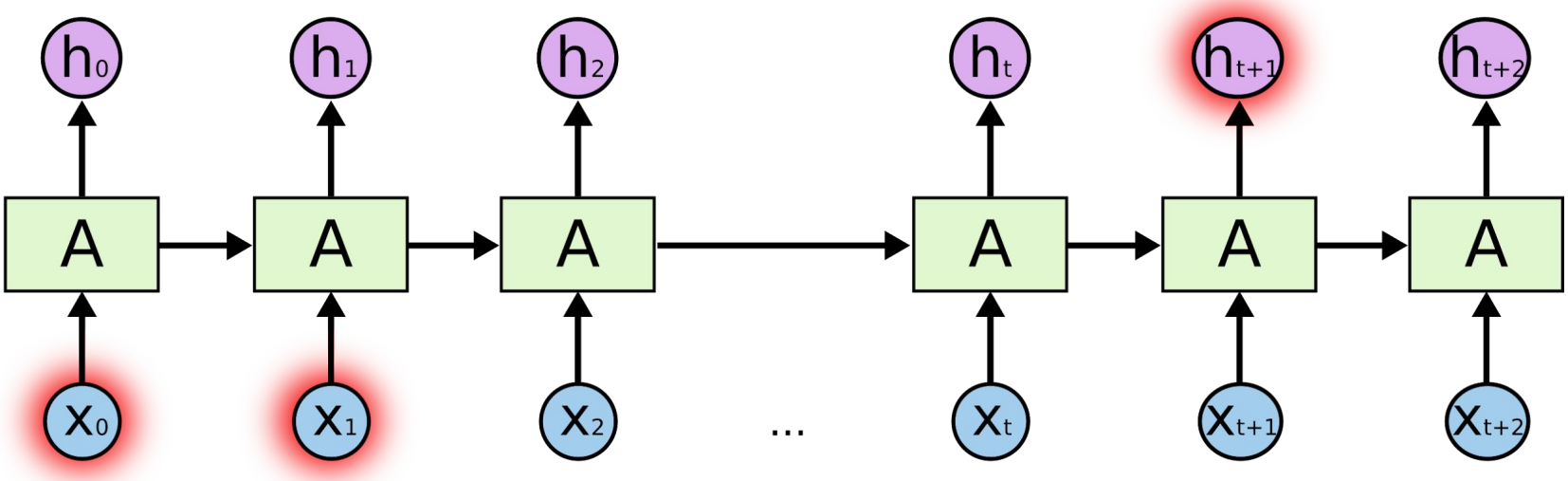
http://colah.github.io/posts/2015-08-Understanding-LSTMs/

RNN refresher



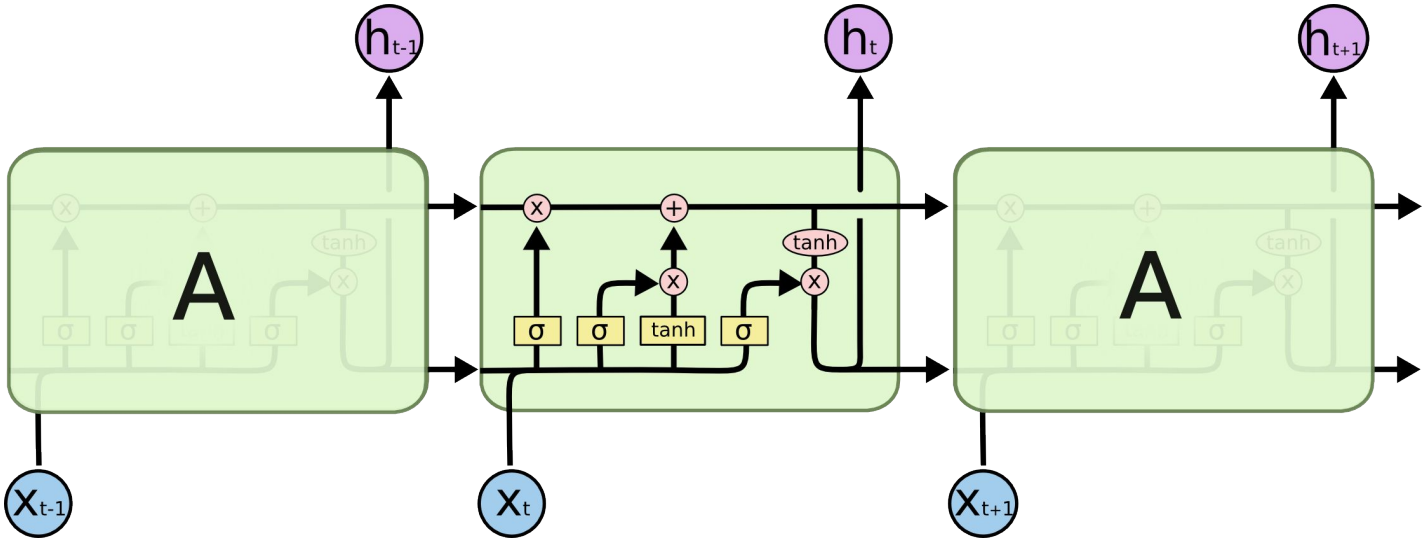
http://colah.github.io/posts/2015-08-Understanding-LSTMs/

RNN refresher



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

LSTM refresher



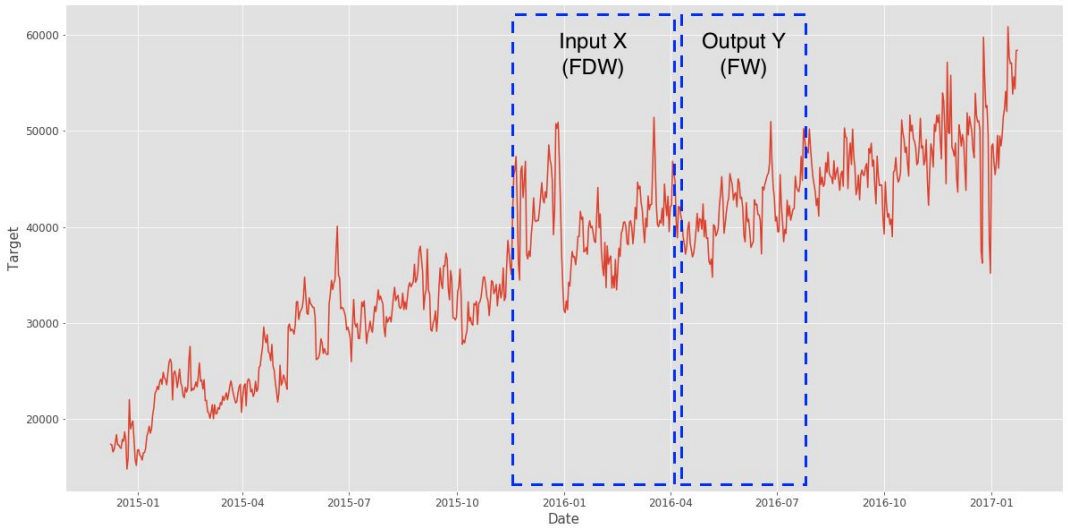
http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Why RNNs for time series

1. Autocorrelated process.
2. Huge success in NLP which is also sequential problem.
3. *Maybe* can do automatic feature extraction and learn hidden patterns in data.
4. *Maybe* can learn trend and seasonality automatically, without special feature engineering.

Preprocessing

Generate sequences of historical data points and sequences of targets.



$[X_1, X_2, X_3, X_4] \rightarrow [y_5, y_6, y_7]$

$[X_2, X_3, X_4, X_5] \rightarrow [y_6, y_7, y_8]$

...

$[X_t, X_{t+1}, X_{t+2}, X_{t+3}] \rightarrow [y_{t+4}, y_{t+5}, y_{t+6}]$

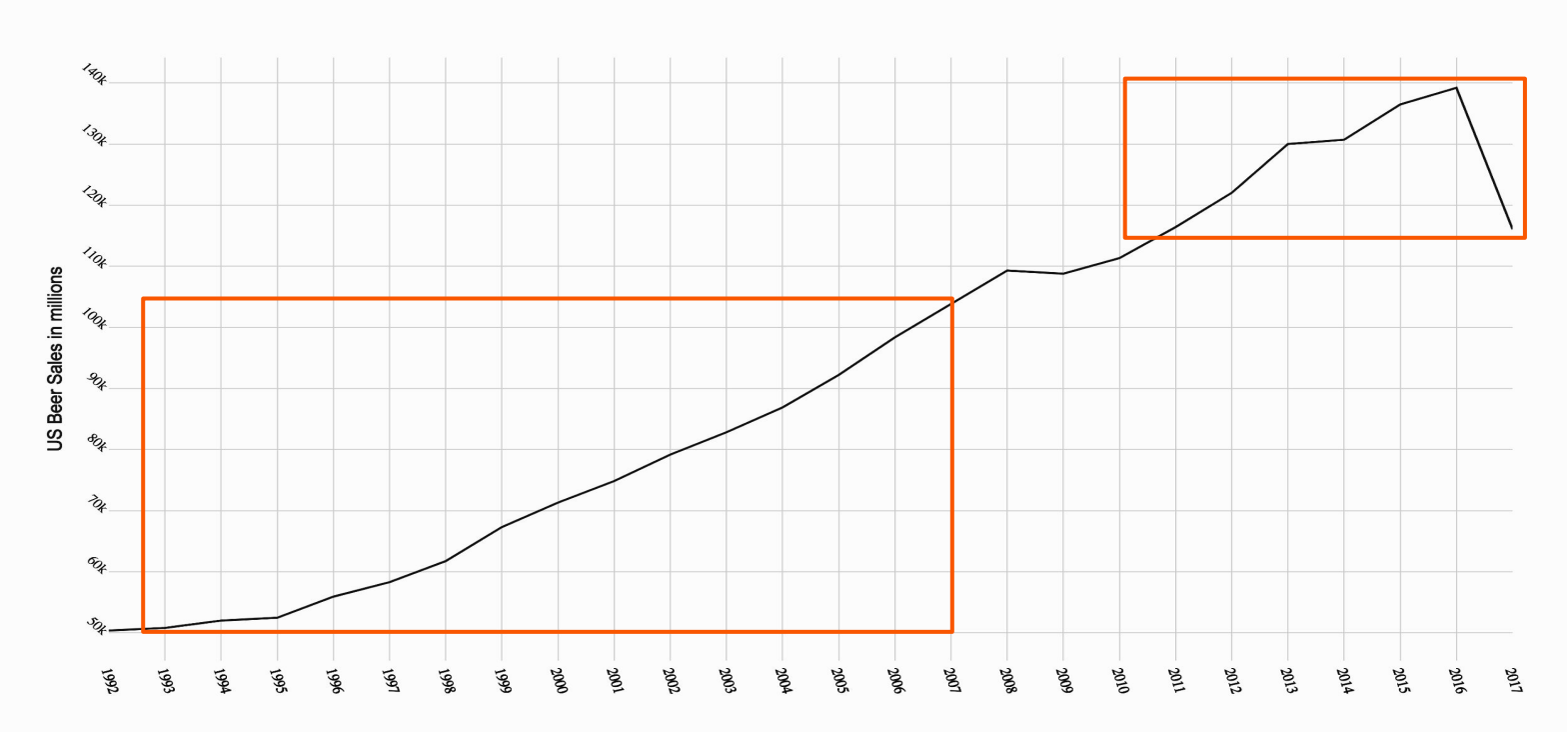
Normalization

Normalization is very important step.

Wrong normalization technique or mistakes can ruin NN performance no matter how sophisticated architecture is.

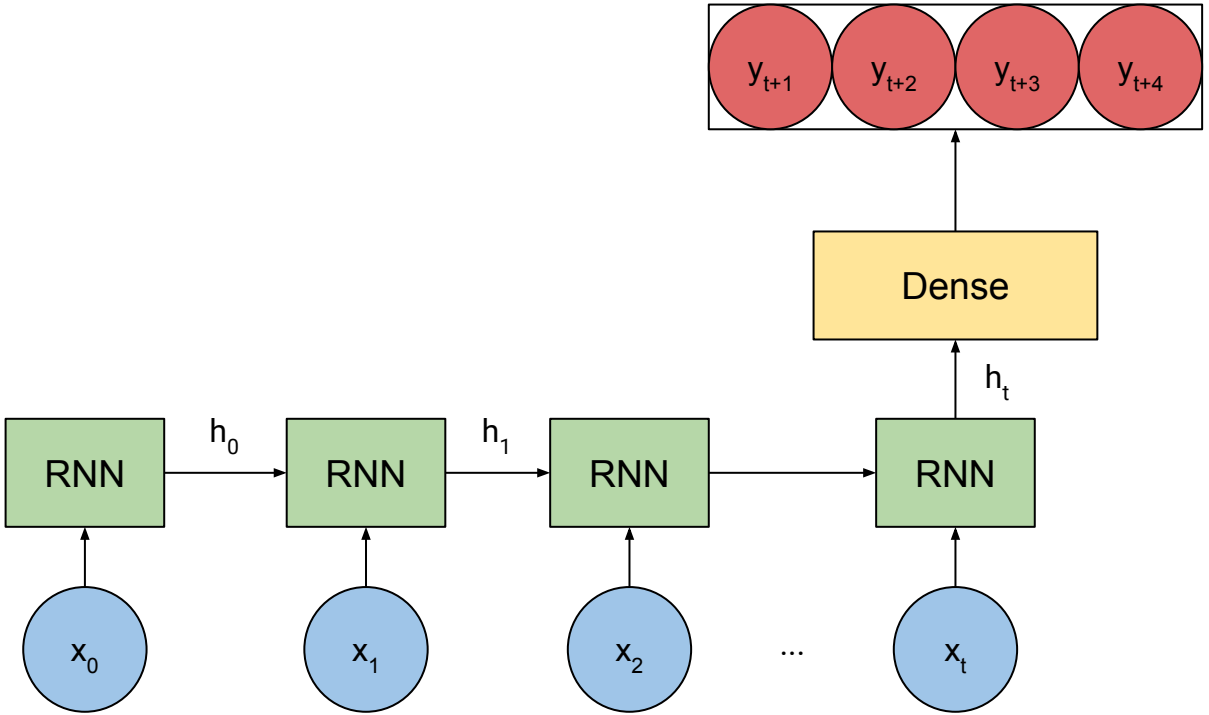
It can be done across all time series, but usually better to do it locally, e.g. divide each sliding window by some value like mean or median. c

Normalization

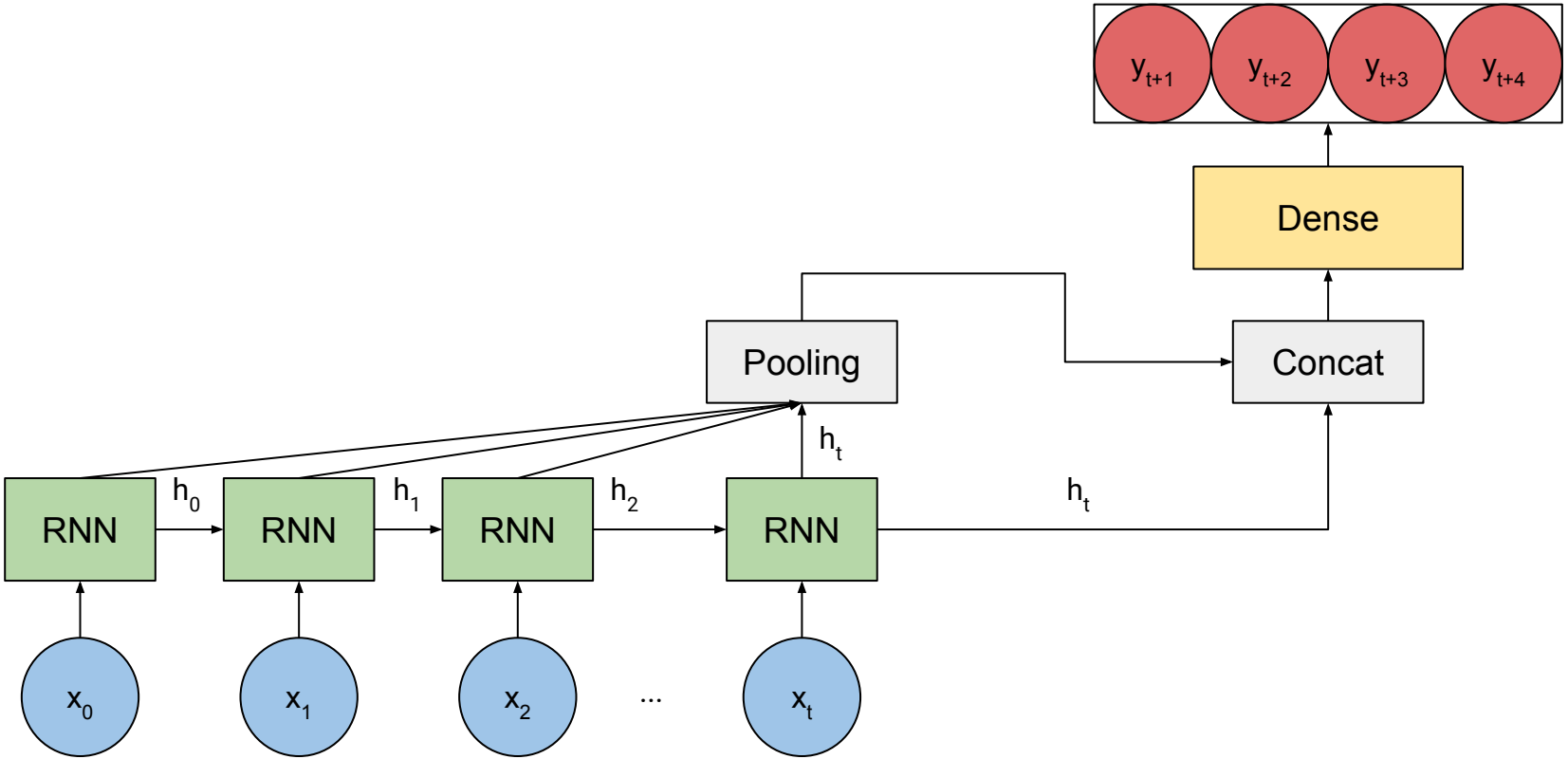


Now let’s talk about models

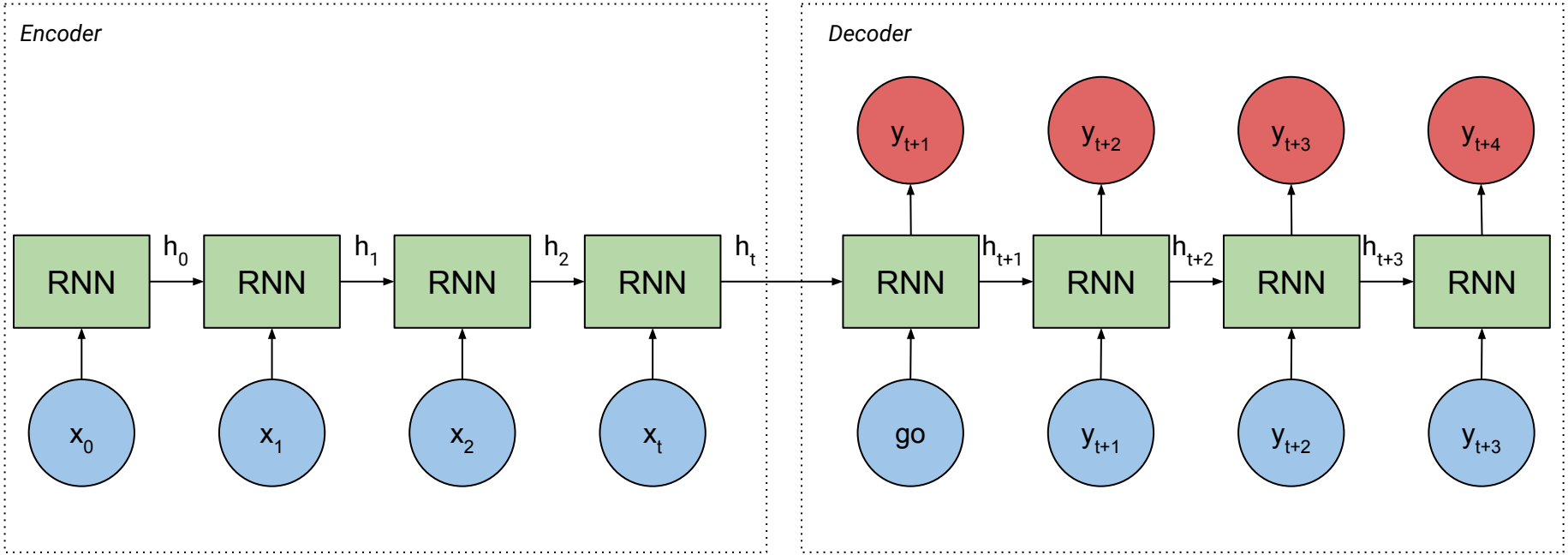
Simple LSTM architecture



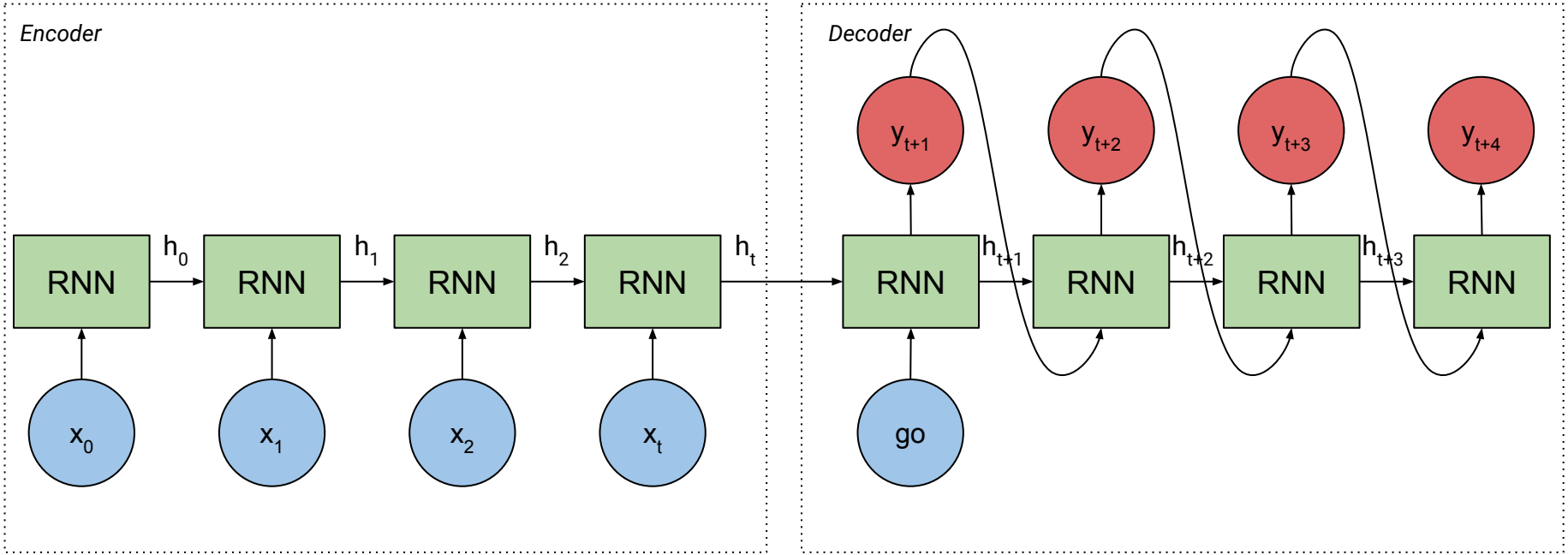
Improvement: use all hidden states



Sequence to sequence



Sequence to sequence (prediction)



Feature preprocessing

Numerical

Missing values imputation & normalization

Categorical & Series ID

Categorical embedding or one-hot encoding

A priori

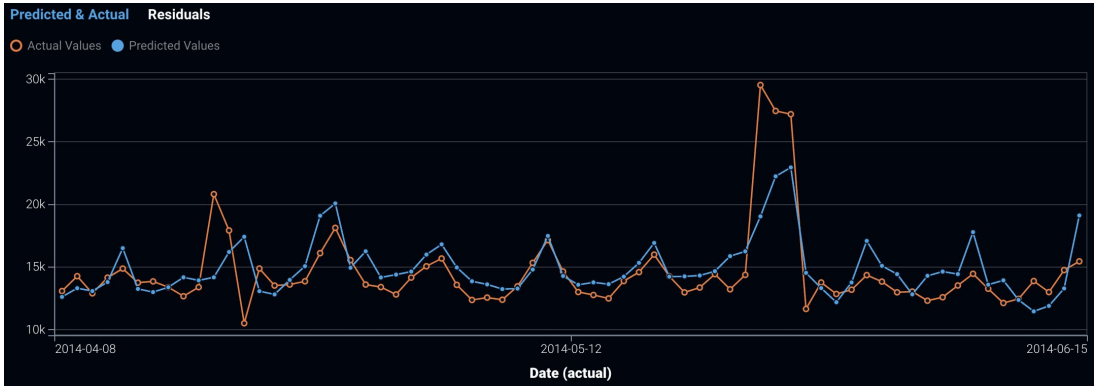
According to type, but also feed into network separately

A priori features

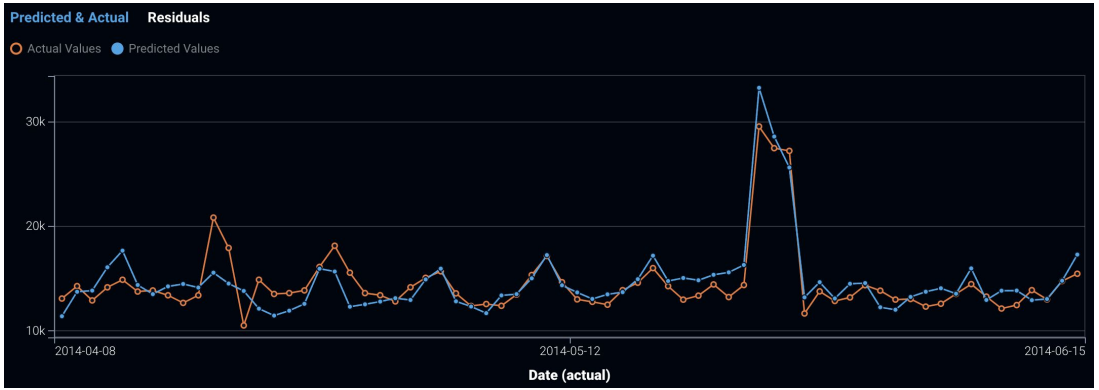
Features, which are known in advance, at the time of prediction.

For example, whether prediction date is a Holiday is known upfront, or whether store is going to do marketing campaign for an item.

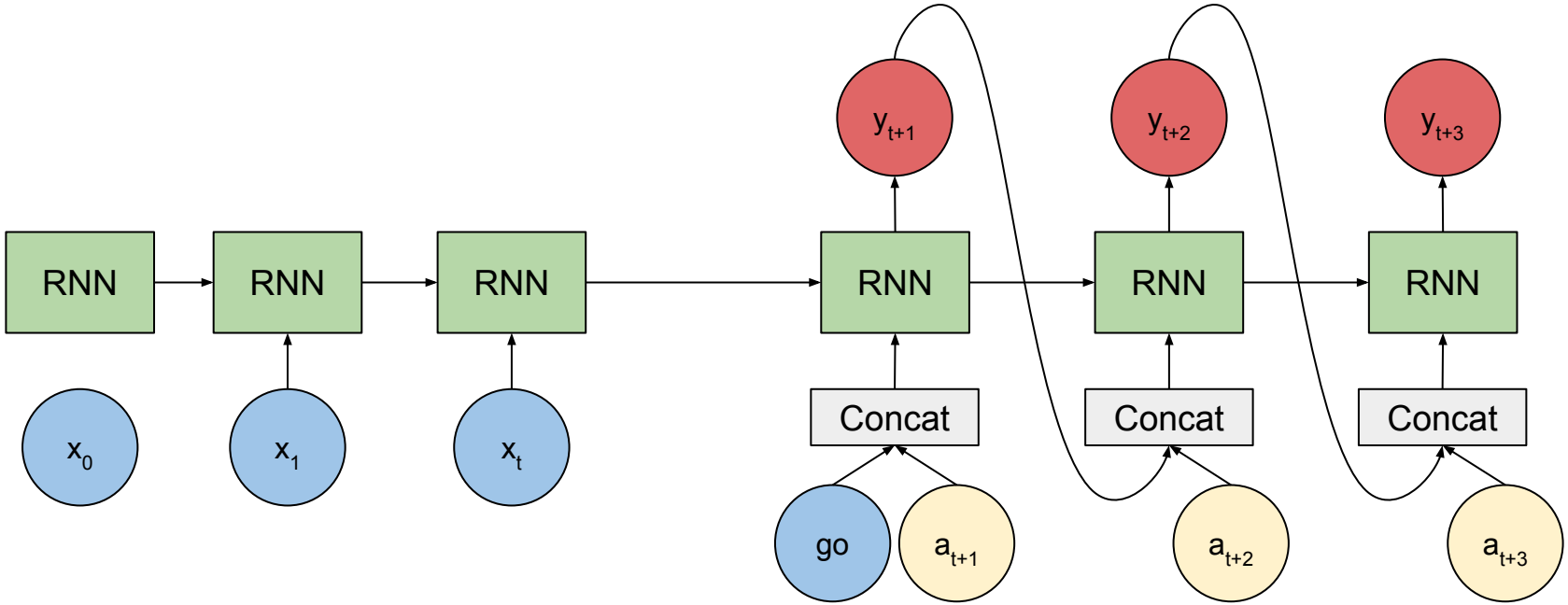
Without a priori features



With a priori features



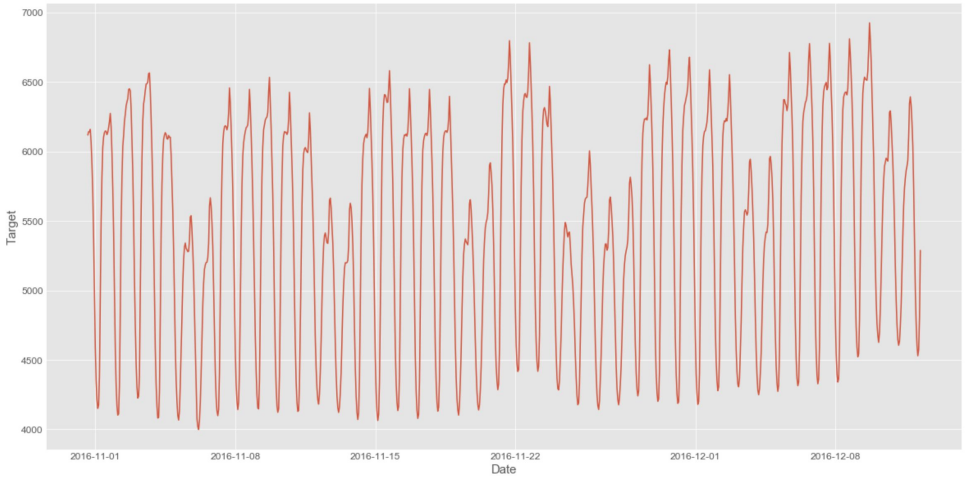
Sequence to sequence with a priori features



Exercise

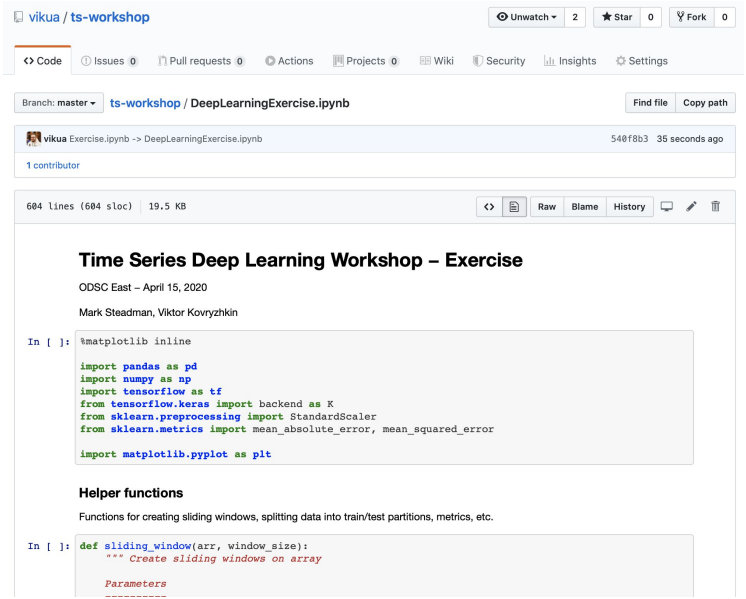
Setup:

- Hourly dataset of energy consumption on NYC
- Multiple seasonalities - intraday and intraweek
- FDW (X): 168 hours (7 days)
- FW (Y): 24 hours
- Model: LSTM seq2seq



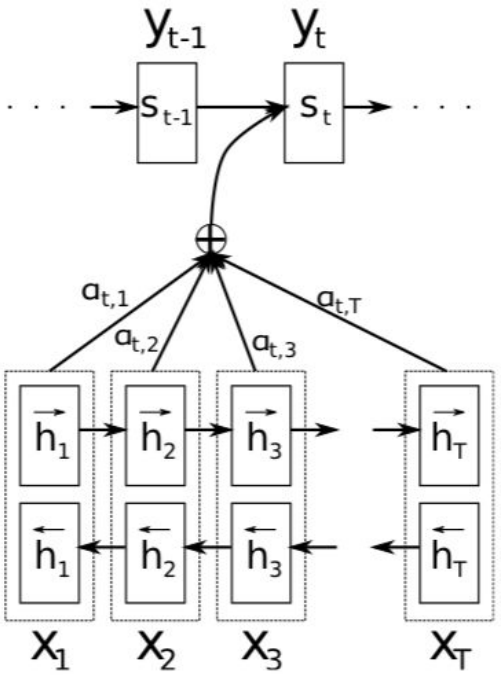
Exercise

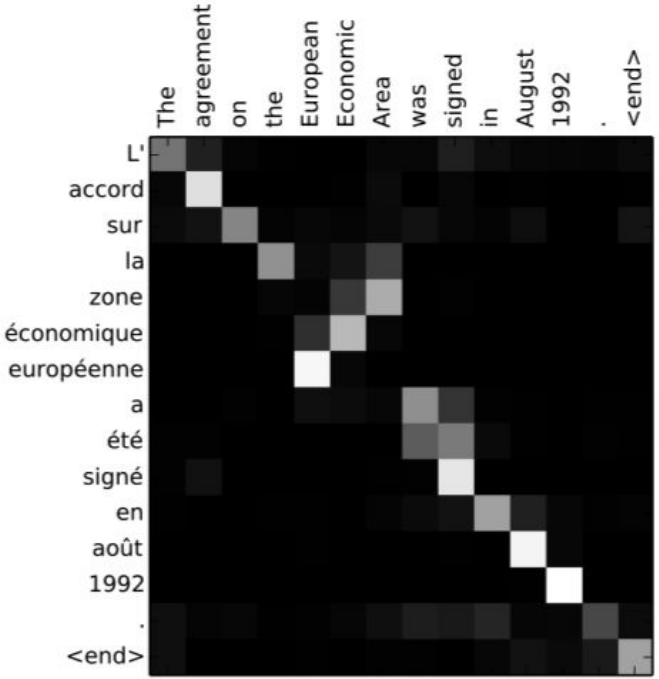
Walkthrough in Python



https://github.com/vikua/ts-workshop

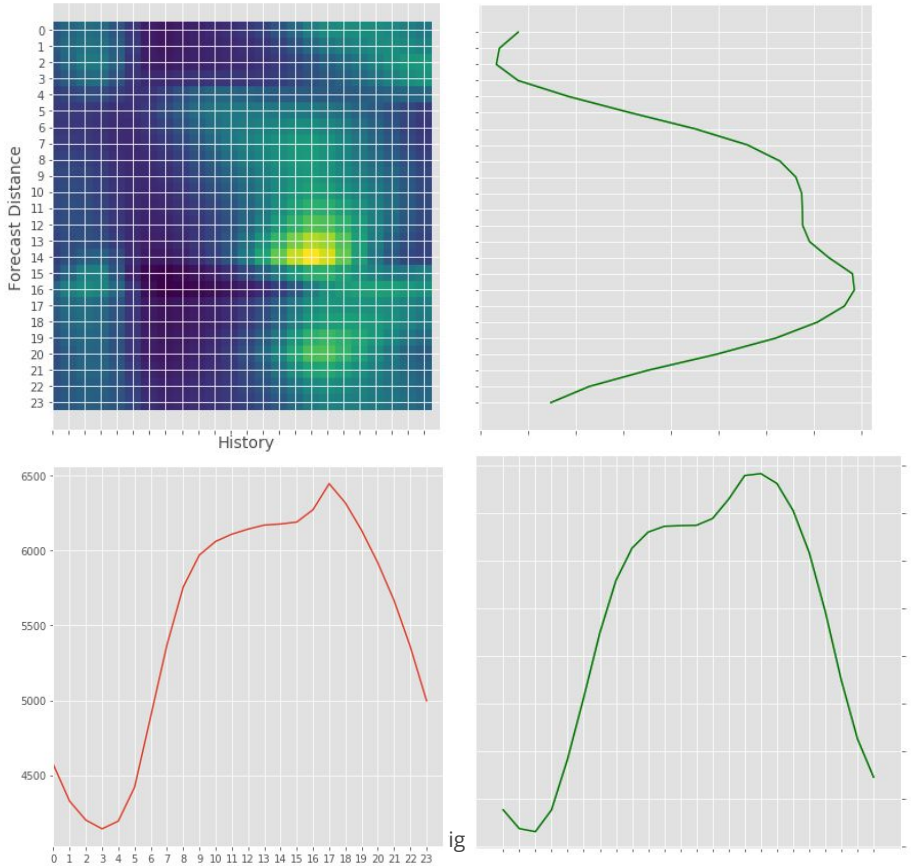
Attention





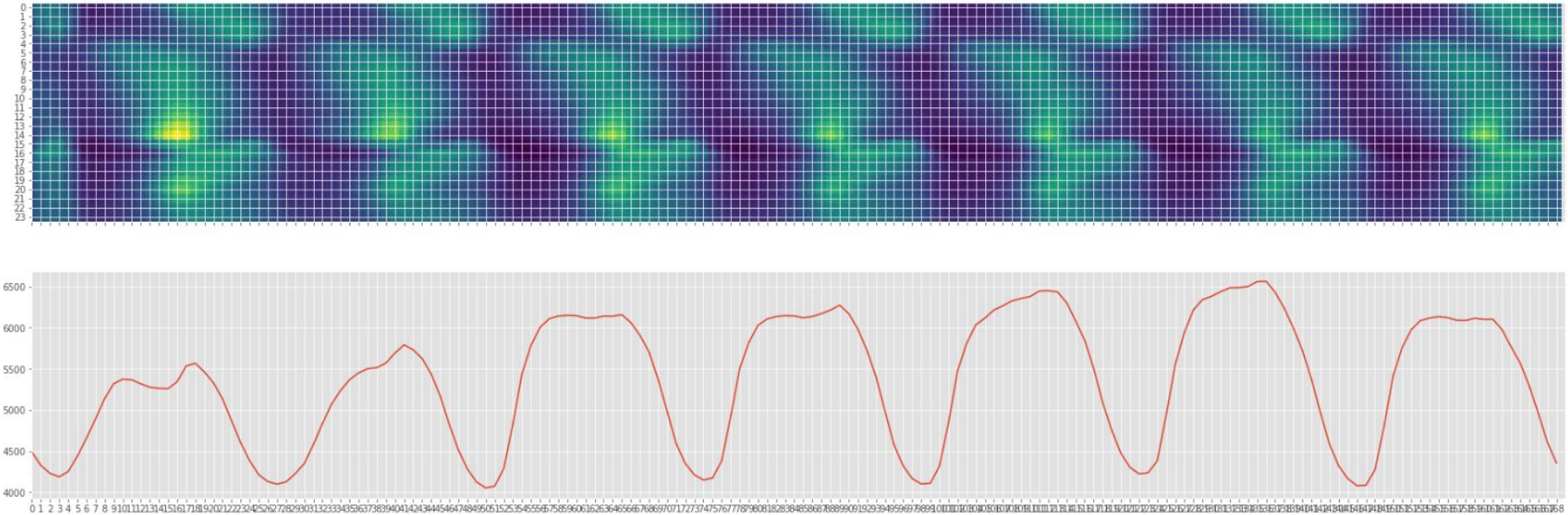
https://arxiv.org/abs/1409.0473

Attention

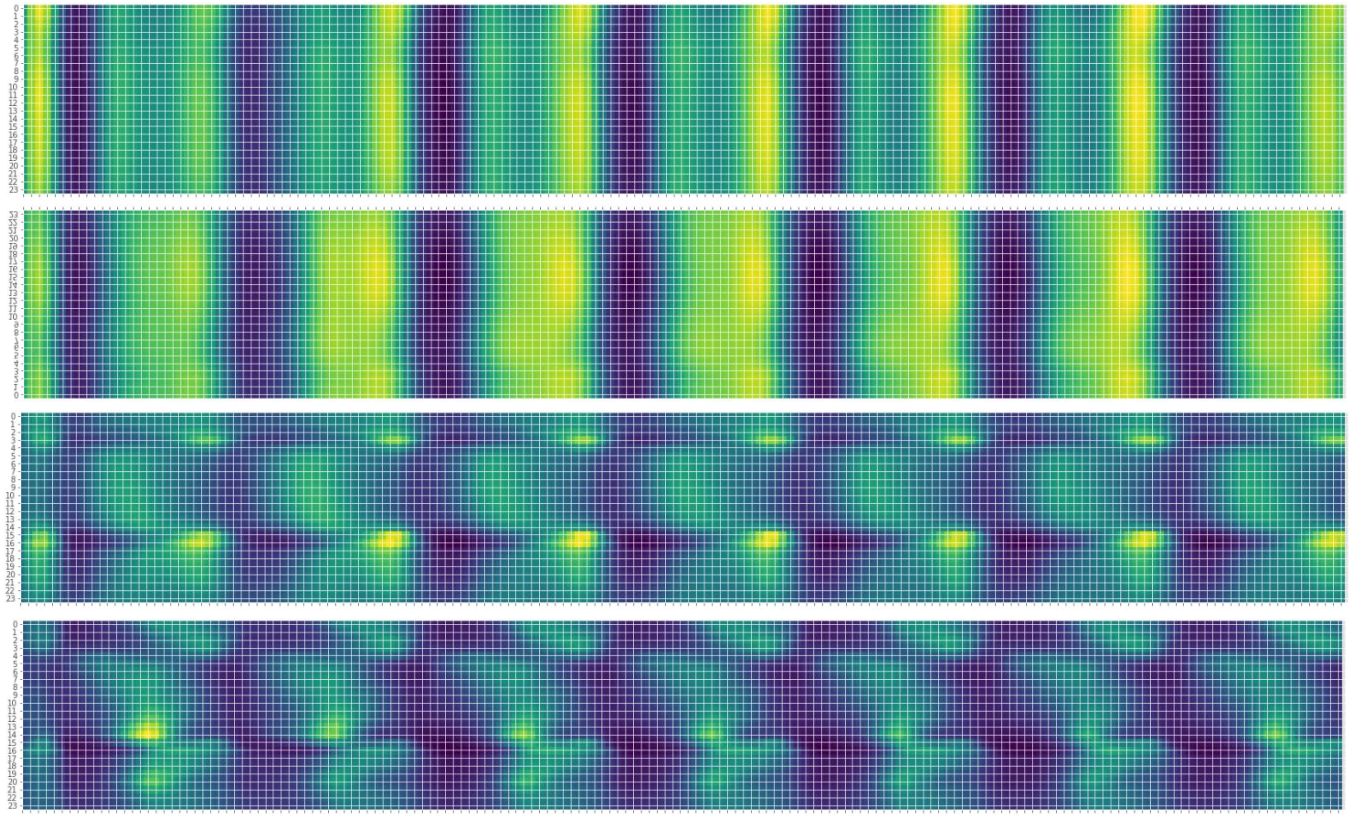


https://arxiv.org/abs/1409.0473

Attention weight (univariate model)



Attention weight (univariate model)



5 epochs

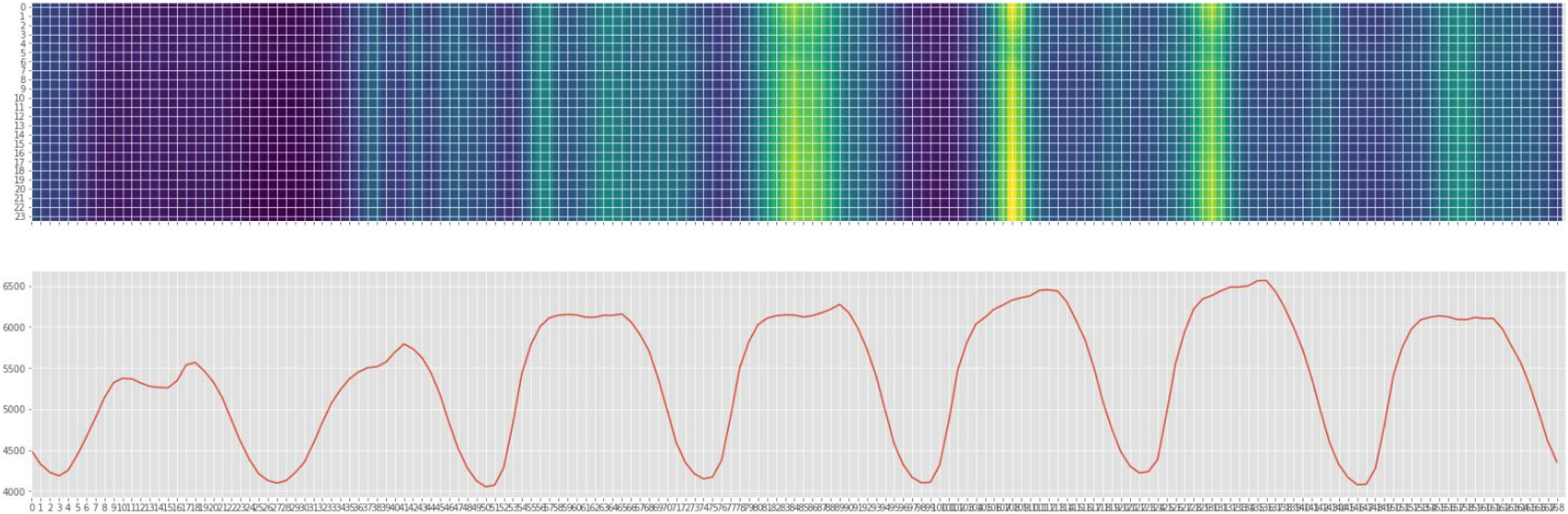
10 epochs

20 epochs

50 epochs

Attention weight (multivariate model)

With more predictive features attention doesn't make that much of a sense



Other architectures

ES-RNN	First place winning solution in M4 competition (by Uber)
DeepAR	https://docs.aws.amazon.com/sagemaker/latest/dg/deepar.htm
Deep state space models	https://papers.nips.cc/paper/8004-deep-state-space-models-for-time-series-forecasting
Auto-encoders for feature extraction	https://eng.uber.com/neural-networks/

Automation

Key requirements to automate this process

- Time series data and framework
- Target transformations
- Feature generation
- Feature reduction
- Standard data preparation
- Model generation and validation