Forecasting Big Time Series: Old and New

Tutorial for VLDB, 2018

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CMU/**Amazon Research** and **AWS AI Labs**




https://lovvge.github.io/Forecasting-Tutorial-VLDB-2018/

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aws Carnegie Mellon VLDB2018

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Forecasting Big Time Series: Old and New

1. Introduction to Forecasting
2. Classical approaches (local, learning one time series at a time)
3. Modern approaches (globally finding patterns)
4. Building forecasting systems

Out of Scope, but we still want to point it out ...

Pattern finding, outlier/anomaly detection, modeling, forecasting and similarity indexing are closely related:

- For forecasting, we need to estimate
  - patterns/rules/models
  - similar past settings
- For outlier/anomaly detection, we can use forecasts
  - outlier = too far from our forecast

Reference

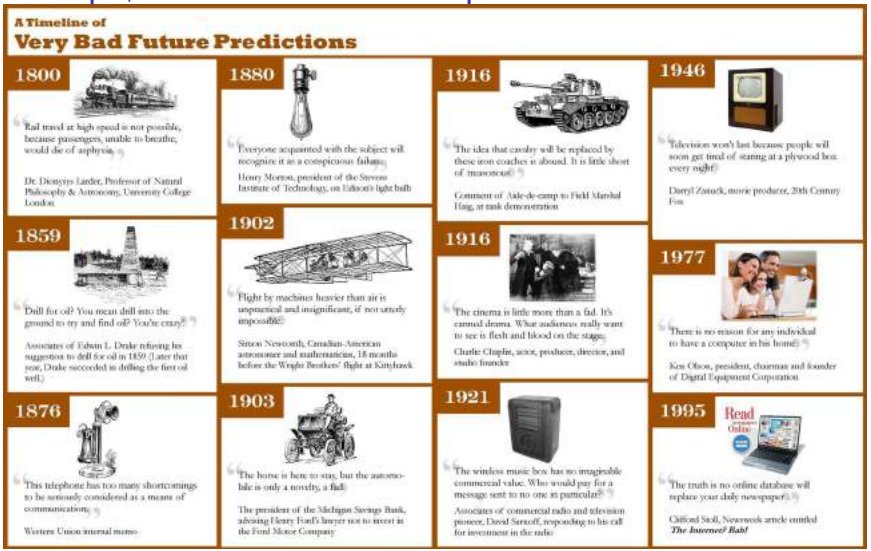


Smart Analytics for Big Time-series Data

Yasushi Sakurai, Yasuko Matsubara and Christos Faloutsos

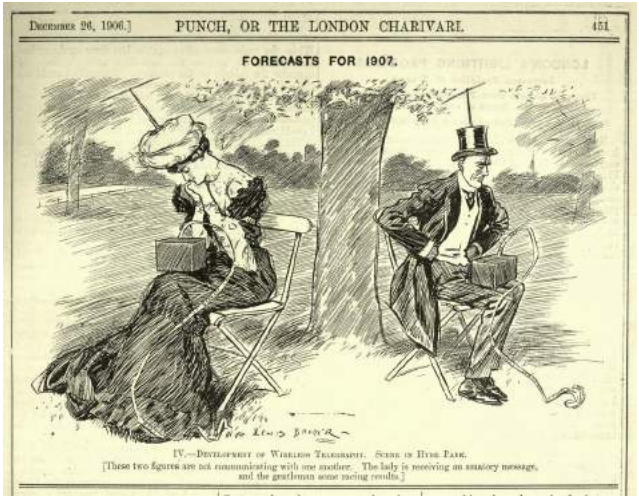
http://www.cs.kumamoto-u.ac.jp/~yasukoTALKS/17-KDD-tut/

Within the Scope, but we still want to point it out ...



http://infographic.city/timeline-bad-future-predictions/

Within the Scope, but we still want to point it out ...



Forecast for 1907:
Telegraph kills live communication!

First Principle

Forecasts are always wrong.

https://medium.freecodecamp.org/worst-tech-predictions-of-the-past-100-years-c18654211375

Within the Scope, but we still want to point it out ...

Prediction is very difficult, especially about the future. – Niels Bohr

Within the Scope, but we still want to point it out ...

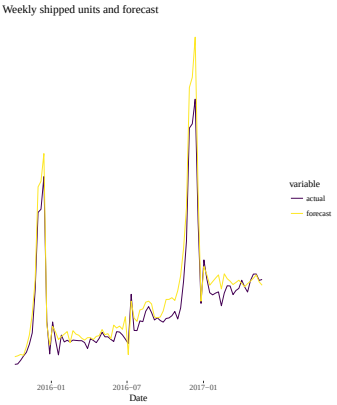
Prediction is very difficult, especially about the future. – Niels Bohr

Second Principle

Whenever possible, formulate the problem in a different way.

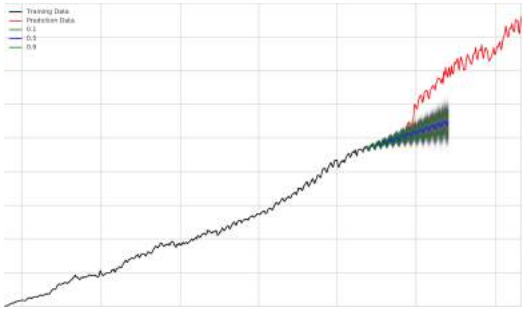
Introduction to Forecasting: Old and New

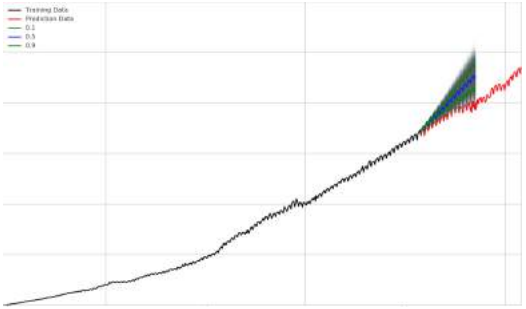
Forecasting Problems at Amazon I: Retail Demand



- Problem: predict overall Amazon retail demand years into the future
- Decision Problems: topology planning, market entry/segment analyses

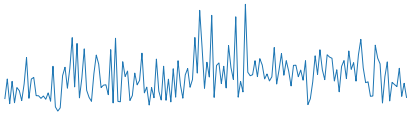
Forecasting Problems at Amazon II: AWS Compute Capacity

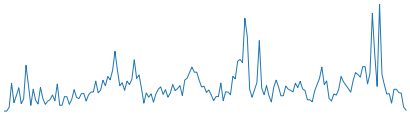




- Problem: predict AWS compute capacity demand
- Decision Problem: how many servers to order when and where

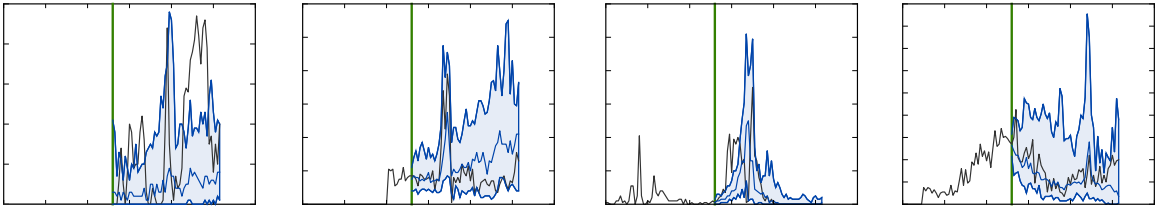
Forecasting Problems at Amazon III: Staff Planning





- Problem: predict attendance rate of fulfillment center staff
- Decision Problems: how to schedule staff and when to hire how much staff

Forecasting Problems at Amazon IV: Retail Product Forecasting



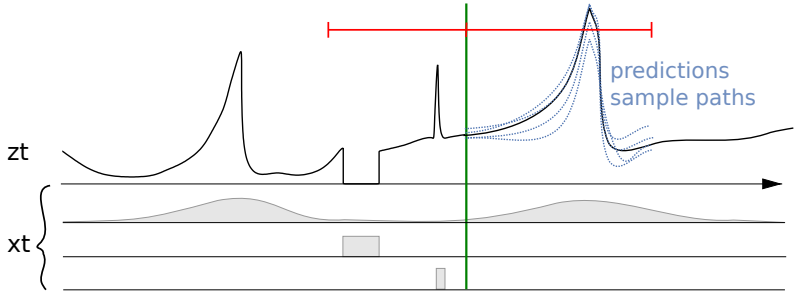
- Problem: predict the demand for a each product available on Amazon
- Decision Problems: how many units to order when and where, when to mark products down

What is Forecasting?

Australian beer shipments: weekly time series (07 Jan 1970 to 05 Dec 1973)

http://www.broo.com.au/australian-beers

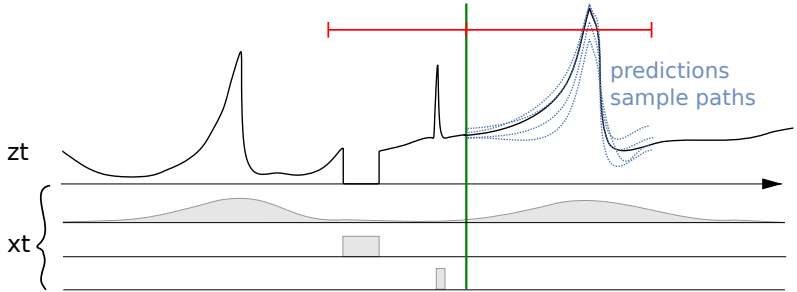
Forecasting Problems: General Setup



- Predict the future behavior of a (univariate) time series $z_{i,t}$ for item $i \in I$ given its past

$$z_{i,0}, \ldots, z_{i,T-2}, z_{i,T-1}, z_{i,T} \Longrightarrow P(z_{i,T+1}, z_{i,T+2}, \ldots z_{i,T+h})$$

Forecasting Problems: General Setup



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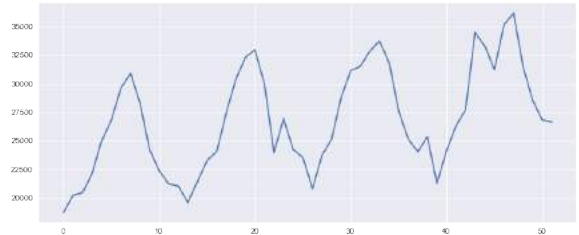
- Make optimal decisions

$$\text{best action} = \underset{a}{\operatorname{argmin}}\, \mathrm{E}_{\mathrm{P}}[\text{cost}(a, z_{i,T+1}, z_{i,T+2}, \ldots z_{i,T+h})]$$

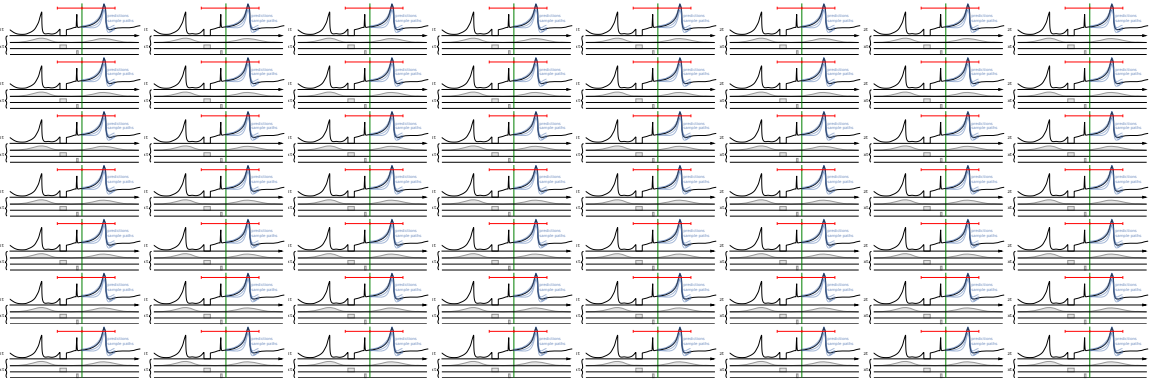
Forecasting Problems: Old and New



- small number of time series
- sufficient historical data
- limited meta data
- hand-crafted models
- statistician and econometrician heavy

We refer to these problems as strategic forecasting problems.

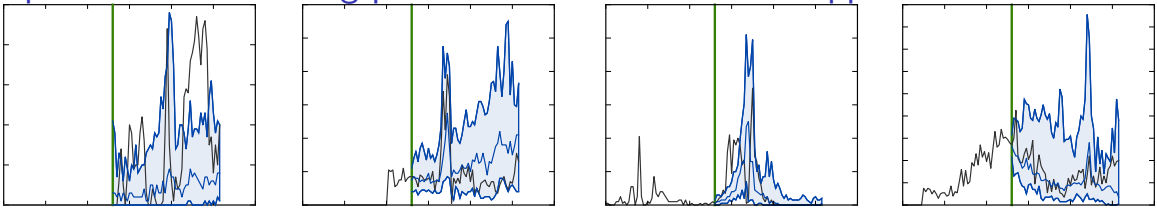
Forecasting Problems: Old and New



Examples: demand for products of a retailer, work force cohorts of a company in its locations, compute capacity needs per region and server type.

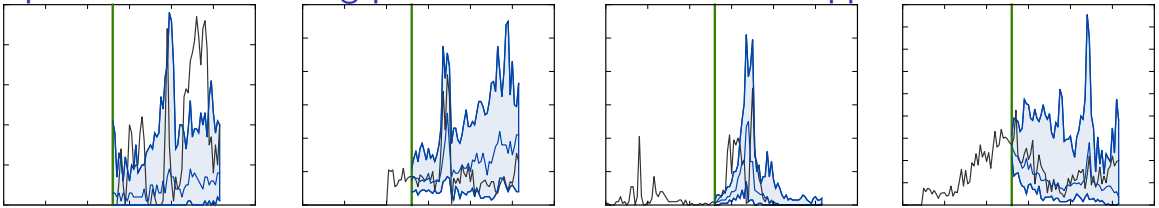
We refer to these problems as operational forecasting problems.

Operational forecasting problems: characteristics & approaches



- cold start/new items
- short cycles
- burstiness, sparsity
- high degree of automation of downstream systems
- ratio of people/time series $\ll 1$

Operational forecasting problems: characteristics & approaches



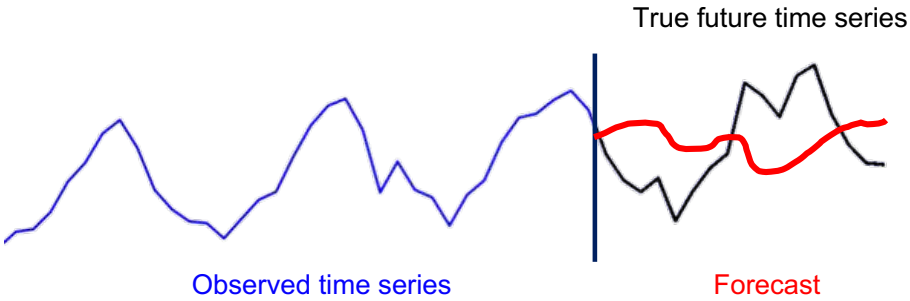
- cold start/new items
- short cycles
- burstiness, sparsity
- high degree of automation of downstream systems
- ratio of people/time series $\ll 1$

Two extremes (to be covered in Part 5):

- complex pipeline of simple models (adapt traditional models to new problems)
- simple pipeline including end-to-end learning with complex models

Metrics to Evaluate Point Forecast

Metrics to Evaluate Point Forecast



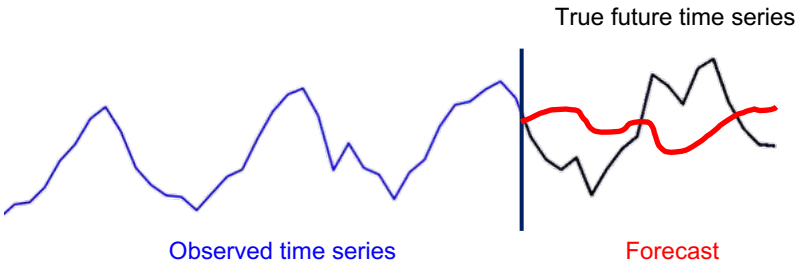
Absolute Error : $e_t = |z_t - \widehat{z}_t|$

- Mean Absolute Error (MAE): mean(e_t) (over forecast horizon h)
- Mean Absolute Percentage Error (MAPE): $\frac{1}{h}\sum_t e_t / |z_t|$
- Root Mean Square Error (RMSE): $\sqrt{\text{mean}(e_t^2)}$

From Point Forecasts to Probabilistic Forecasts

To paraphrase George E. P. Box

All forecasts are wrong, but some are useful ...



Point forecasts are typically insufficient for decision making.

$$\text{best action} = \underset{a}{\operatorname{argmin}}\, \mathrm{E}_{\mathrm{P}}[\text{cost}(a, z_{i,T+1}, z_{i,T+2}, \ldots z_{i,T+h})]$$

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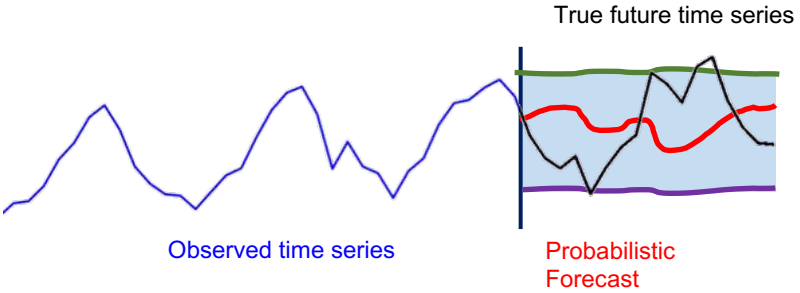

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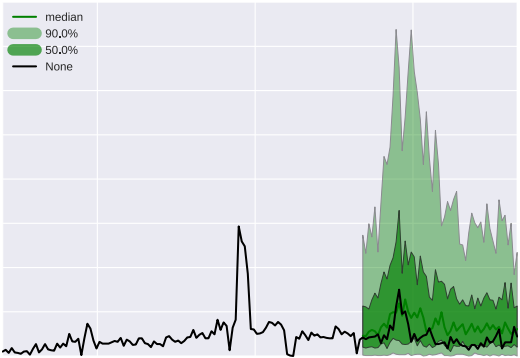
$$\text{best action} = \operatorname*{argmin}_{a} \mathrm{E}_{\mathrm{P}}[\text{cost}(a, z_{i,T+1}, z_{i,T+2}, \ldots z_{i,T+h})]$$

From Point Forecasts to Probabilistic Forecasts

Probabilistic Forecast

What is the distribution of the future time series values $P(\widehat{z}_t)$?

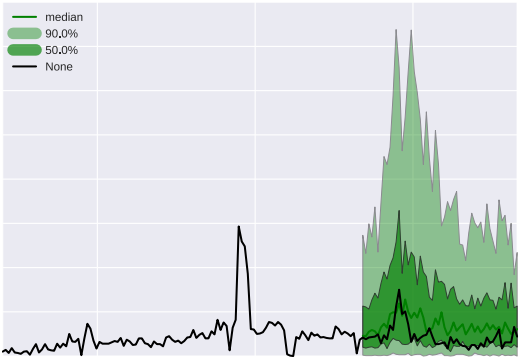


- P50 Forecast: 50% of the time $z_t \leq \widehat{z}_t$
- P90 Forecast: 90% of the time $z_t \leq \widehat{z}_t$

Evaluating Probabilistic Forecast

Probabilistic Forecast

P90 forecast means 90% of the time the true value $z_t \leq \hat{z}_t$ (or precisely $\hat{z}_t^{0.9}$)



Quantile Loss

$$e_t^q = \begin{cases} q \cdot (z_t - \hat{z}_t^q), & z_t \geqslant \hat{z}_t^q \\ (1-q) \cdot (\hat{z}_t^q - z_t), & \hat{z}_t^q \geqslant z_t \end{cases}$$

$\hat{z}_t^q$: Forecast at quantile q

Hit Rate / Calibration

Percentage of $z_t \leqslant \hat{z}_t^q$

Quantile Loss and Calibration: Two Sides of the Coin

Quantiles Loss

P90 forecast means 90% of the time the true value z_t is smaller than the forecast.

$$e_t = \begin{cases} 0.9 \cdot (z_t - \widehat{z}_t), & z_t \geqslant \widehat{z}_t \\ 0.1 \cdot (\widehat{z}_t - z_t), & \widehat{z}_t \geqslant z_t \end{cases}$$

Quantile loss is **proper scoring rule**, which means optimizing this metric leads to an accurate P90 forecast.

Quantile Loss and Calibration: Two Sides of the Coin

Calibration

P90 forecast means 90% of the time the true value z_t is smaller than the forecast.

$$(\text{Percentage of } z_t \leqslant \widehat{z}_t) \approx 90\%$$

Calibration alone is not enough ...

True target time series	5, 5, 5, 5, 5, ...
P50 Forecast	0, 100, 0, 100, 0, 100, ...

Perfectly calibrated (calibration = 50%), but horrible forecast ...

Probabilistic Forecast

Goal

The goal of probabilistic forecasting is to maximize the sharpness of the predictive distribution subject to calibration. [Gneiting et al., 2007]

- Sharpness: the width of the predictive intervals
- The forecast distribution should be as close as possible to the true distribution

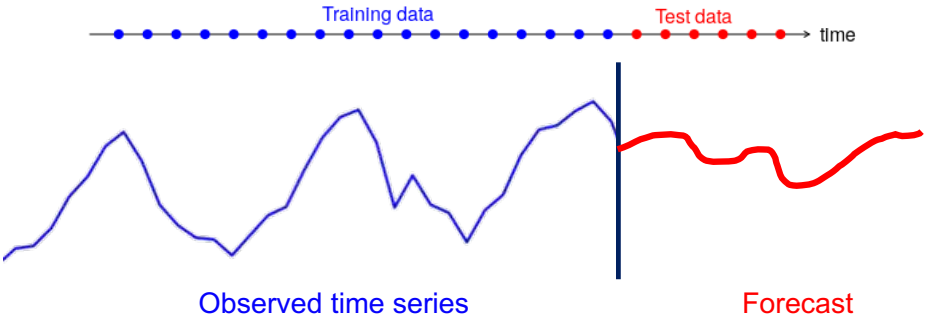
Continuous Ranked Probability Score (CRPS)

$$\text{CRPS} = \int_0^1 \text{QUANTILE LOSS}(q)\mathrm{d}q$$

Optimizing CRPS leads to sharp and calibrated forecast.

Evaluating Forecasts: Backtesting

Compute forecast accuracy on observed data for a fixed time series i:



Evaluating Forecasts: Backtesting

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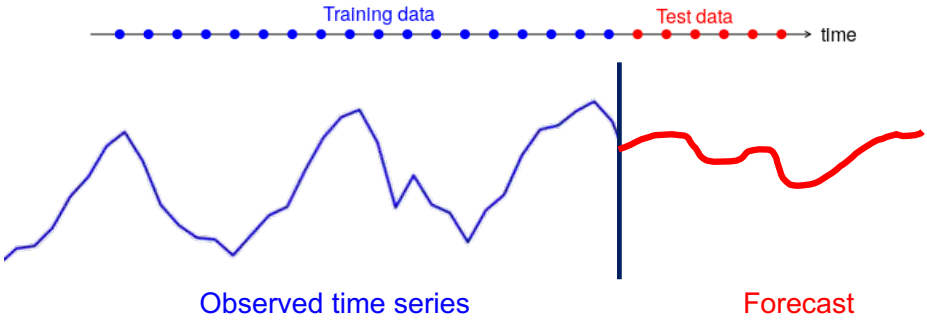

Accuracy now depends on the start of test data.

Evaluate forecast: better backtesting

Compute forecast accuracy (to be defined) on observed data for a fixed time series i:

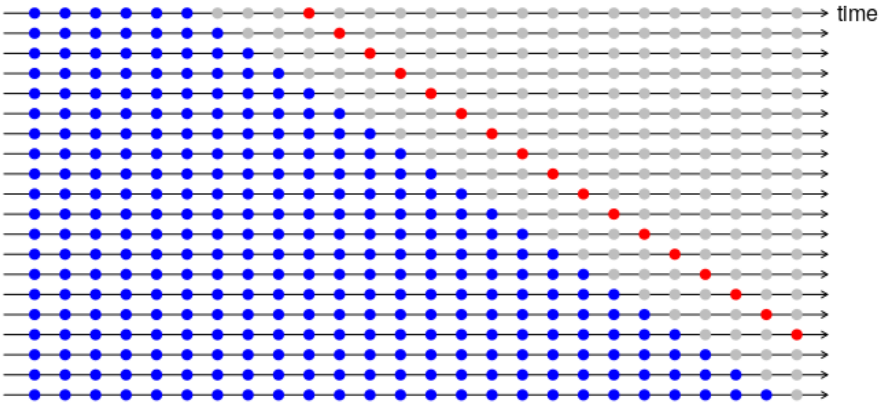

Figure: [Hyndman and Athanasopoulos, 2017]

Some Remarks on Accuracy

Alternative to MAPE, we can introduce scale-independent accuracy by scaling using

- the error of a benchmark/standard method (e.g., MRAE)
- the forecast accuracy of a benchmark method (e.g., RelMAE)
- in-sample random walk (e.g., MASE)
- evaluating spatio-temporal forecast with Optimal Transport [Roberts et al., 2017]

More in [Hyndman and Koehler, 2006; Kolassa and Schuetz, 2007]

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More in [Hyndman and Koehler, 2006; Kolassa and Schuetz, 2007]

Practical subtleties:

- how to evaluate given missing values (e.g., out-of-stock situations, errors in recording of events)?
- deal with $\cdot/0$ and $0/0$

Some Remarks on Accuracy

Potentially three different accuracy measures:

- loss-function for training the model
- forecast accuracy metric for backtesting
- forecast accuracy measure for reporting to stakeholders

Metric needs to be simple, intuitive. Insist on it being a proper score.

Some Remarks on Accuracy

Potentially three different accuracy measures:

- loss-function for training the model
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Metric needs to be simple, intuitive. Insist on it being a proper score.

Crucial to understand the down-stream consequences of the forecasts:

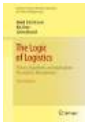
$$\text{best action} = \underset{a}{\operatorname{argmin}}\, \mathrm{E}_{\mathrm{P}}[\text{cost}(a, z_{i,T+1}, z_{i,T+2}, \ldots z_{i,T+h})]$$

More accurate forecasts may not lead to better downstream decisions.

Selected References

[Makridakis et al., 1998]. Classic introductory book.

[Hyndman and Athanasopoulos, 2017]. Recent introductory book.

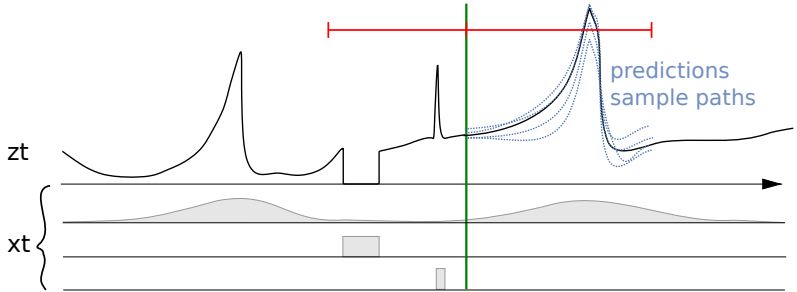


[Larson et al., 2001; Simchi-Levi et al., 2013]. Introduction to practical Supply Chain problems including forecasting.

General business forecasting journal:
https://foresight.forecasters.org/

Classical Methods for Forecasting: Old and New

Forecasting Problems: General Setup



- Predict the future behavior of a time series z_i for item $i \in I$ given its past

$$\ldots, z_{i,T-2}, z_{i,T-1}, z_{i,T} \Longrightarrow P(z_{i,T+1}, z_{i,T+2}, \ldots z_{i,T+h})$$

- Make optimal decisions

$$\text{best action} = \underset{a}{\operatorname{argmin}}\, \mathrm{E}_{\mathrm{P}}[\text{cost}(a, z_{i,T+1}, z_{i,T+2}, \ldots z_{i,T+h})]$$

We drop the item index i whenever the context is clear.

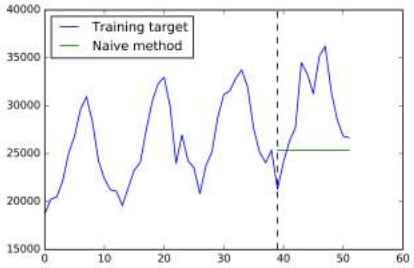
Simple Forecasting Methods

- Input: a sequence of observations $z_1, z_2, \ldots, z_T$
- Output: forecasts for all time steps in forecast horizon h: $T+1, T+2, \ldots, T+h$

Simple Forecasting Methods

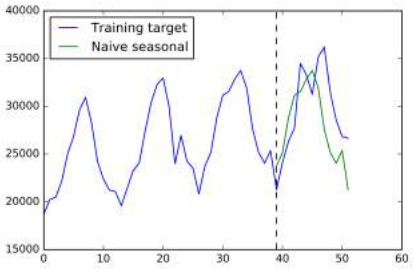
- Input: a sequence of observations $z_1, z_2, \ldots, z_T$
- Output: forecasts for all time steps in forecast horizon h: $T+1, T+2, \ldots, T+h$
- Naive method: future forecasts are equal to the last observed value.

$$z_{T+t} = z_T, \quad t = 1, 2, \ldots, h$$



Simple Forecasting Methods (contd.)

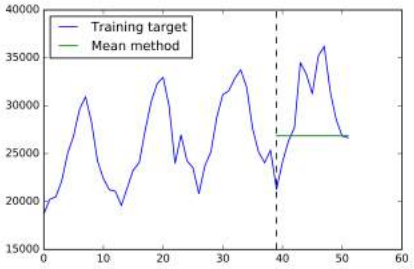
- Naive seasonal method: future forecasts are equal to the observed value from last season.



Simple Forecasting Methods (contd.)

- Mean method: future forecasts are equal to the average of all observed values.

$$z_{T+t} = \frac{1}{T}(z_1 + z_2 + \ldots + z_T), \quad t = 1, 2, \ldots, h$$

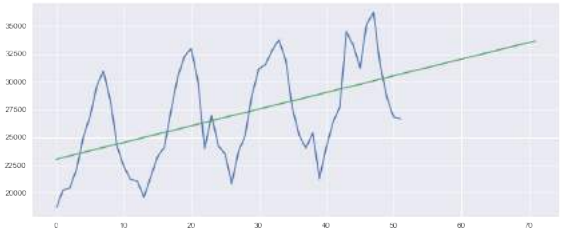


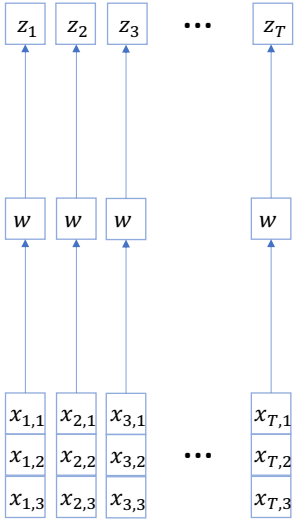
Forecasting with Linear Regression

- Assume our prediction $\widehat{z}_t$ is a weighted combination of *features* $x_{t,1}, \ldots, x_{t,D}$,

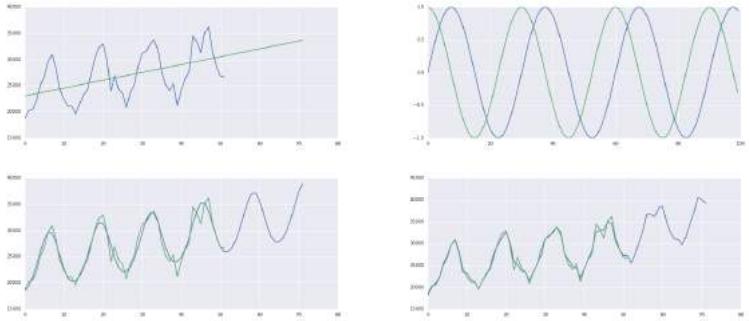
$$\widehat{z}_t = \sum_{d=1}^{D} w_d x_{t,d}$$

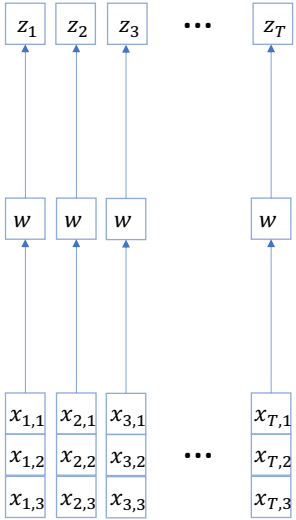
- The features $x_{t,d}$ are assumed to be given (= hand designed)





Forecasting with Linear Regression





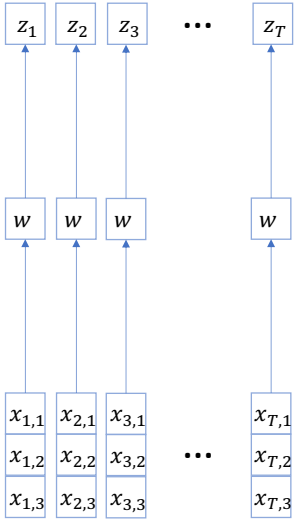
Forecasting with Linear Regression

- Goal: find weights $w_1, \ldots, w_D$ so that our prediction $\widehat{z}_t$ is close to the true z_t.
- Least-squares finds an optimal $w^\star$ by minimizing

$$w^\star = \operatorname*{argmin}_w \sum_{t=1}^{T} (z_t - \widehat{z}_t)^2 = \sum_{t=1}^{T} \left(z_t - \sum_{d=1}^{D} w_d x_{t,d} \right)^2$$

- $w^\star$ can then be used to make forecasts:

$$z_t = \sum_{d=1}^{D} w_d^\star x_{t,d} \qquad t = T+1, \ldots, T+h$$



Features for Linear Regression

The features used in such a linear model are themselves time series $x_{1,d}, x_{2,d}, \ldots, x_{T+H,d}$.

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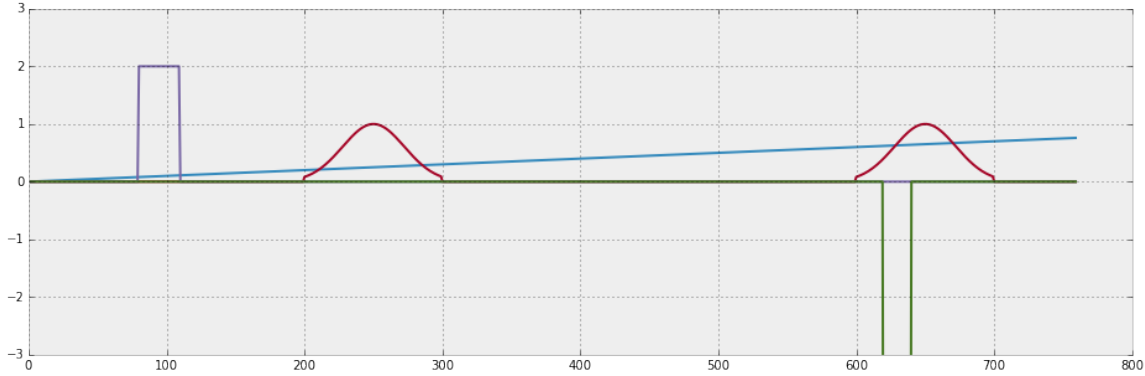

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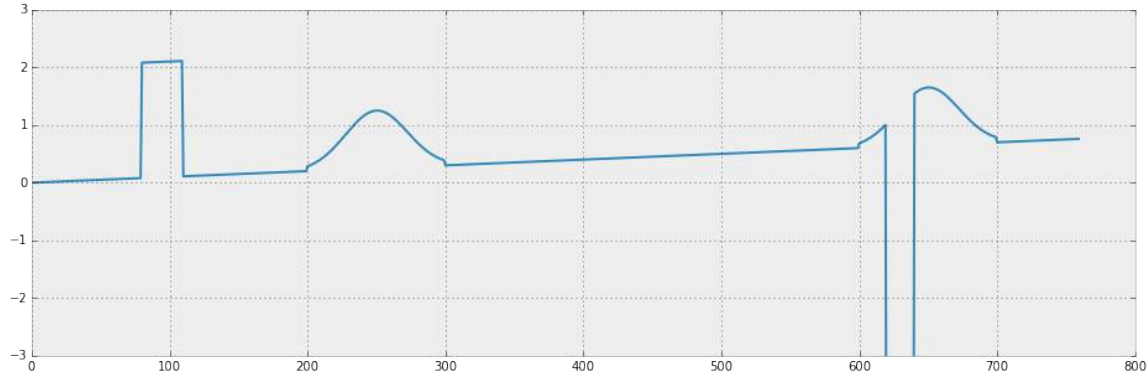
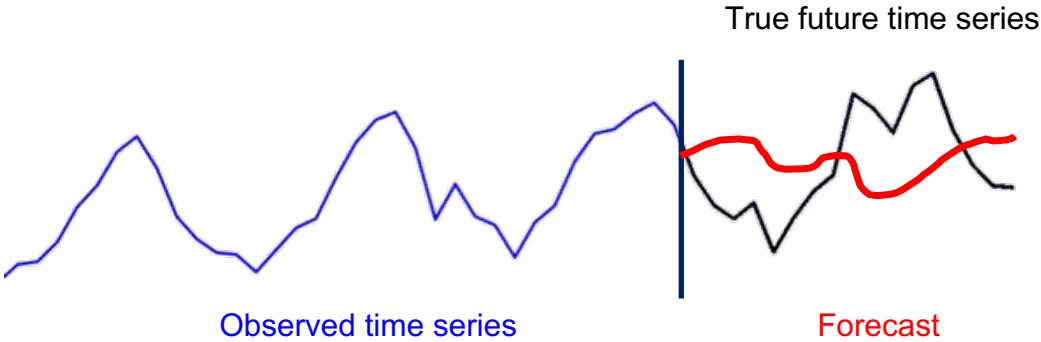


From Algorithm to Probabilistic Model

It is far better to foresee even without certainty than not to foresee at all.
– Henri Poincaré

From Algorithm to Probabilistic Model

$$\min \sum_t e_t, \text{ with } e_t = (\widehat{z}_t - z_t)^2 \Longleftrightarrow \max \prod_t P(e_t), \text{ with } e_t \sim \mathcal{N}(e_t|0, \sigma^2)$$



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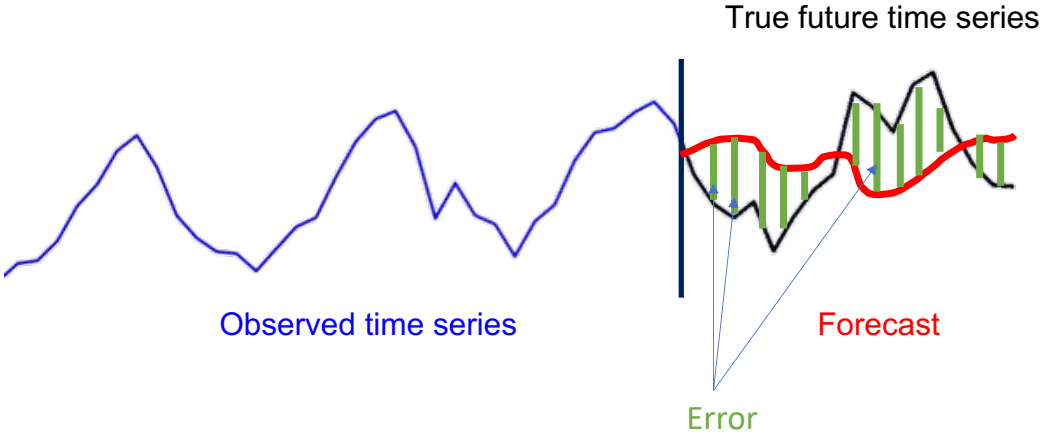

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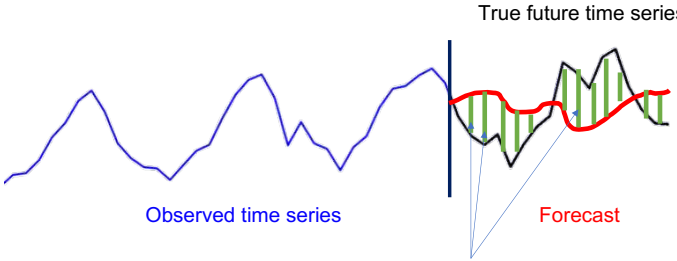

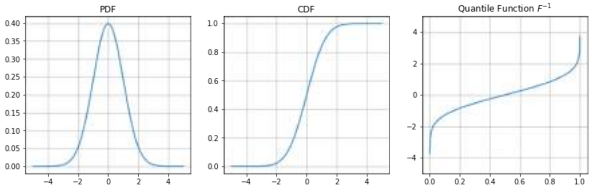

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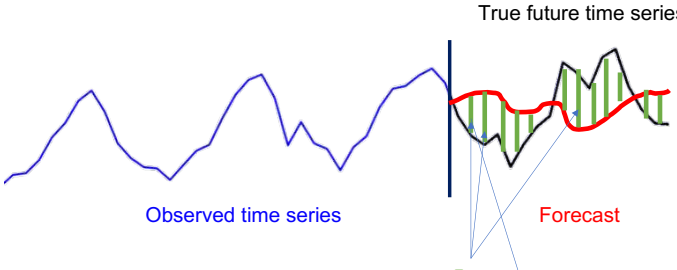

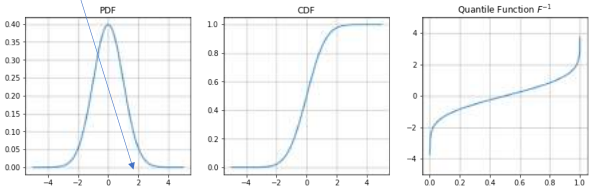

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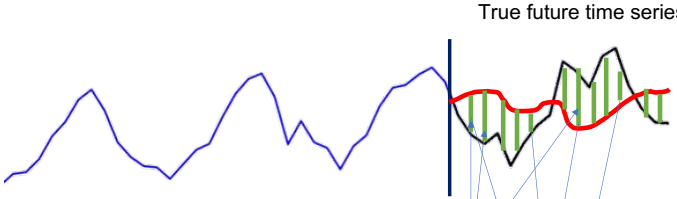
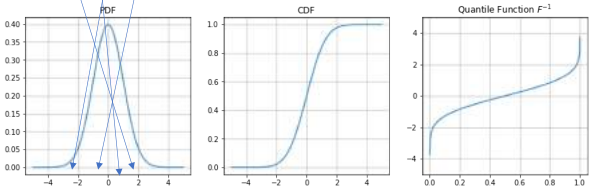




Linear Regression as a Probabilistic Model

- Assume the following *model* for the data, introducing a *latent* (unobserved) variable y_t

$$y_t = \sum_{d=1}^{D} w_d x_{t,d}$$
$$z_t = y_t + \epsilon_t \qquad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

- Equivalently, $P(z_t|y_t) = \mathcal{N}(z_t|y_t, \sigma^2)$, so that

$$P(z_t|y_t) = \mathcal{N}(z_t|y_t, \sigma^2) = \mathcal{N}(e_t|0, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{e_t^2}{2\sigma^2}\right\}$$

- In terms of the features $x_{t,d}$ we have

$$P(z_t|x_t) = \mathcal{N}\left(z_t \middle| \sum_d w_d x_{t,d}, \sigma^2\right)$$

Linear Regression as a Probabilistic Model

- Finding the least square solution $w^\star \Longrightarrow$ maximum likelihood estimation (MLE)

$$
\begin{aligned}
w^\star &= \underset{w}{\operatorname{argmax}} \prod_{t=1}^{T} P(z_t|x_t) = \underset{w}{\operatorname{argmax}} \sum_{t=1}^{T} \log P(z_t|x_t) \\
&= \underset{w}{\operatorname{argmax}} \sum_{t=1}^{T} \left(-\log \sqrt{2\pi\sigma^2} - \left(z_t - \sum_d w_d x_{t,d} \right)^2 / (2\sigma^2) \right) \\
&= \underset{w}{\operatorname{argmax}} \sum_{t=1}^{T} - \underbrace{\left(z_t - \sum_d w_d x_{t,d} \right)^2}_{e_t^2} \\
&= \underset{w}{\operatorname{argmin}} \sum_{t=1}^{T} e_t^2
\end{aligned}
$$

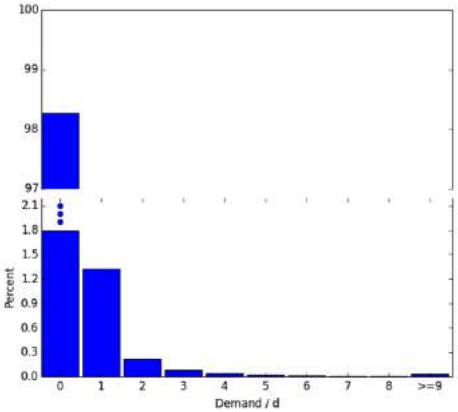
- We can also find the optimal σ^2 in the same way

Generalized Linear Models (GLM)

- The Gaussian noise *assumption* $P(z_t|y_t) = \mathcal{N}(z_t|y_t, \sigma^2)$ is a modelling *choice*!
- Other choices for $P(z_t|y_t)$ (observation model, also called *likelihood* in Bayesian models) are possible
- Common choices are:
  - Poisson, Negative-Binomial (count data)
  - Beta (data in $(0, 1)$ interval)
  - Bernoulli (binary data)
  - Student-t (heavy-tailed real data)

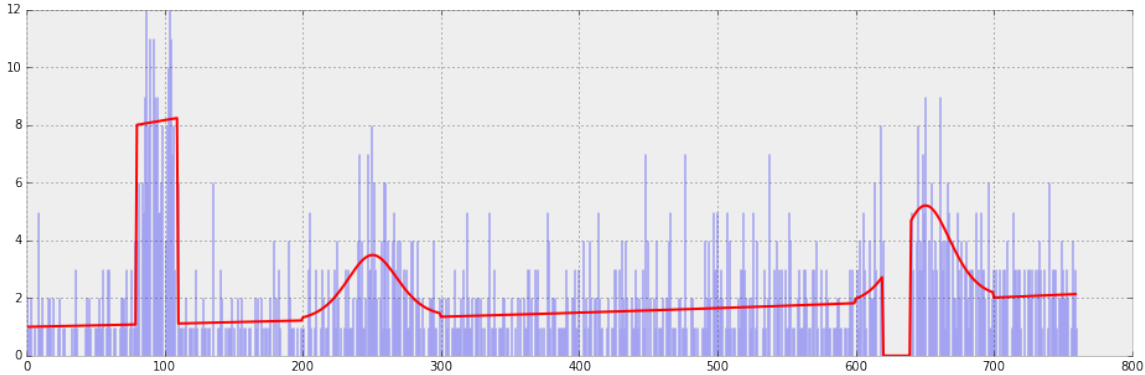
Latent Linear Models: Likelihood $P(z_t|y_t)$

- In daily real-world sales data, 98% of the values are 0



- Could use (not a good fit): Gaussian, Gamma, Poisson, Negative Binomial (NB)
- Better choices: Zero-inflated Poisson/NB, multi-stage likelihood [Seeger et al., 2016]

Examples



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Fewer parameters $\Longrightarrow$ less training data needed! Less prone to overfitting!

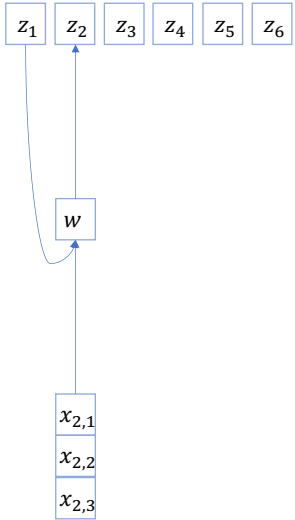
Lagged Target Values / Autoregressive Model

Idea: Use lagged values z_{t-l} (for $l = 1, 2, 3, \ldots, p$) as features to predict z_t

- In a linear model we have $z_t = \sum_d w_d x_{t,d} + b + \epsilon_t$
- By using lagged targets as features, i.e. $x_{t,d} = z_{t-d}$ for $d = 1, 2, \ldots, p$ we get

$$z_t = \sum_{l=1}^{p} w_l z_{t-l} + b + \epsilon_t$$

- Each value is modelled as a weighed average of previous values, plus noise
- The noise is usually assume to be iid. Gaussian, $\epsilon_t \sim \mathcal{N}(0, \sigma^2)$
- This is the so-called **Autoregressive Model (AR)** of order p!



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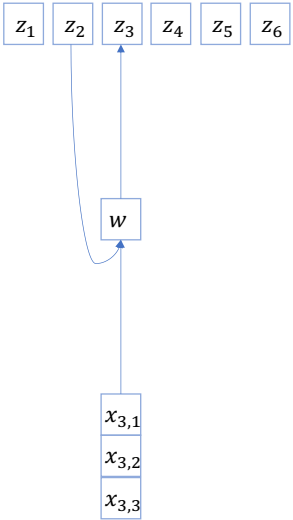

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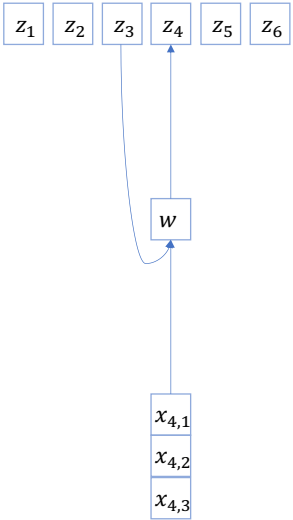

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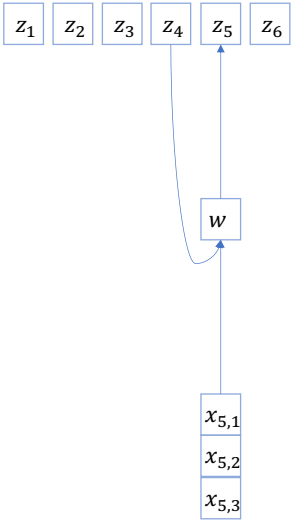

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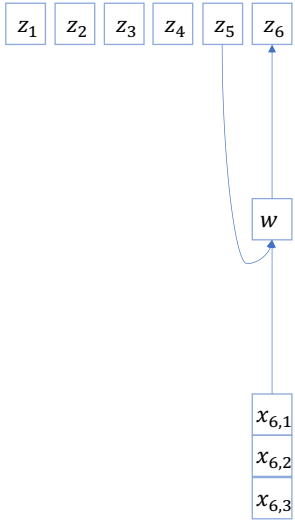

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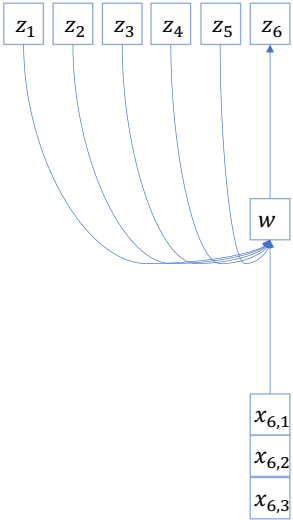
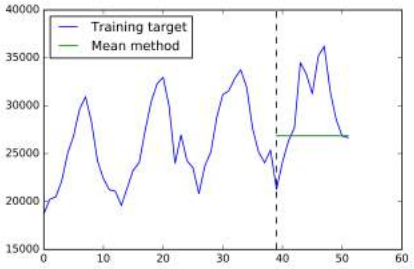


Simple Forecasting Methods: Mean method

- Mean method: future forecasts are equal to the average of all observed values.

$$z_{T+t} = \frac{1}{T}(z_1 + z_2 + \ldots + z_T), \quad t = 1, 2, \ldots, h$$



Alternative to linear regression

Prediction is the weighted average of all observations

$$\widehat{z}_2 = \alpha z_1 + (1-\alpha)\widehat{z}_1$$
$$\widehat{z}_3 = \alpha z_2 + \alpha(1-\alpha) z_1 + (1-\alpha)\widehat{z}_1$$
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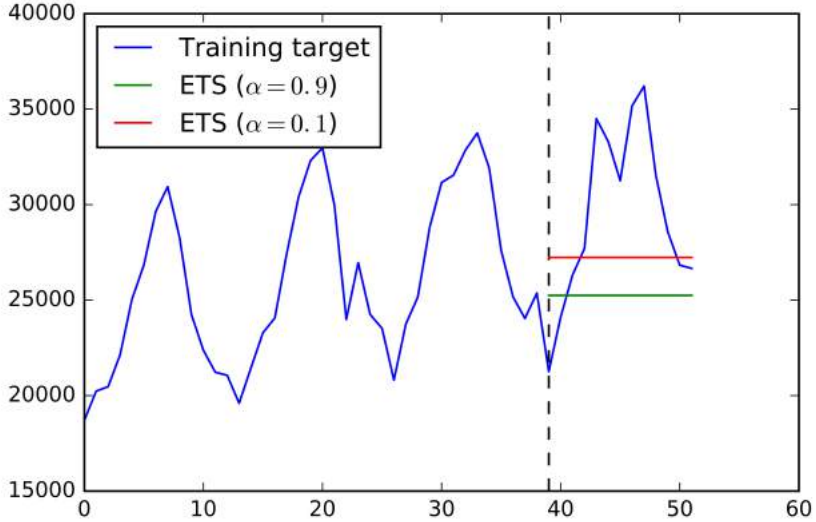
- ETS (Simple ExponenTial Smoothing): weighted average of all observations:

$$\widehat{z}_{T+h} = \alpha z_T + \alpha(1-\alpha)z_{T-1} + \alpha(1-\alpha)^2 z_{T-2} + \dots + (1-\alpha)^T \widehat{z}_1$$

α is a smoothing parameter and $\widehat{z}$ is the prediction for $t = 1$.

ETS (contd.)


Training target
ETS ($\alpha = 0.9$)
ETS ($\alpha = 0.1$)
40000
35000
30000
25000
20000
15000
0
10
20
30
40
50
60

Simple Exponential Smoothing

- Forecast at time t is adjusted to previous error

$$\widehat{z}_{t+1} = \underbrace{\widehat{z}_t}_{\text{previous forecast}} + \alpha \underbrace{(z_t - \widehat{z}_t)}_{\text{error in previous forecast}},$$

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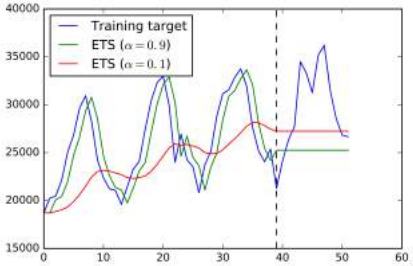

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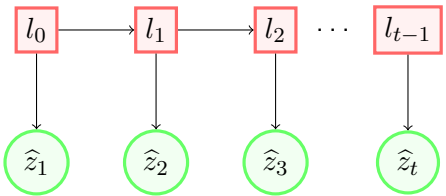
- Latent variable ℓ_t representing the "level" of the time series t

Forecast equation $\quad \widehat{z}_t = \ell_{t-1}$

Error Correction $\quad \ell_t = \ell_{t-1} + \alpha(z_t - \widehat{z}_t),$



- Adjustable parameters: α and ℓ_0

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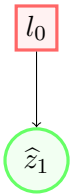

- Adjustable parameters: α and ℓ_0

Simple Exponential Smoothing (contd.)

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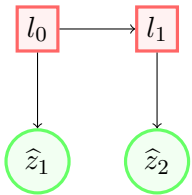

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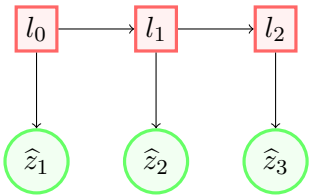

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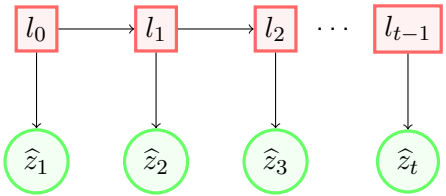

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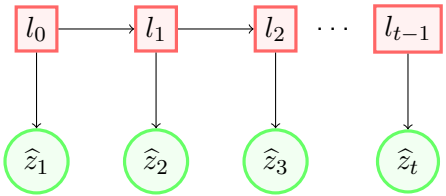

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General Exponential Smoothing

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- $\boldsymbol{a}_t$ $\boldsymbol{F}_t$ depend on the pattern being modeled
- $\boldsymbol{g}_t$ and $\boldsymbol{l}_0$ will be learned from data

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- Statistical model: data generating process
  - produce an entire probability distribution for a future time period
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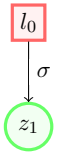

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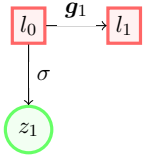

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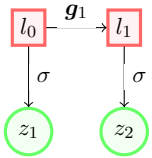

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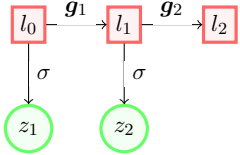

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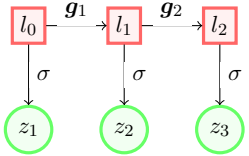

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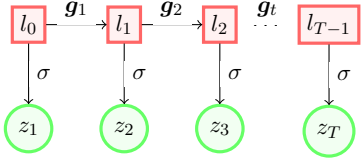

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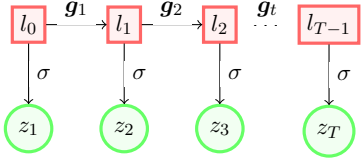

- Parameters: $\boldsymbol{l}_0$, $\boldsymbol{g}_t$ and σ

Linear State Space Models

- Linear dynamical system: $\boldsymbol{l}_t = \boldsymbol{F}\boldsymbol{l}_{t-1} + \boldsymbol{g}\varepsilon_t \qquad \varepsilon_t \sim N(0,1)$
- Encompasses ARIMA and variants of ETS
- Combine linear model and dynamical system to yield

$$z_t \sim P(z_t|y_t)$$
$$y_t = \boldsymbol{x}_t^T \boldsymbol{w} + \boldsymbol{a}^T \boldsymbol{l}_{t-1}.$$
$$\boldsymbol{l}_t = \boldsymbol{F}\boldsymbol{l}_{t-1} + \boldsymbol{g}\varepsilon_t, .$$

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Linear State Space Model part:

$$u_t = \boldsymbol{a}_t^T \boldsymbol{l}_{t-1}$$

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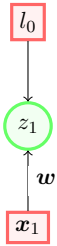

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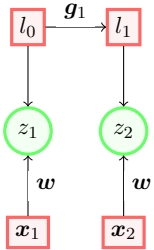

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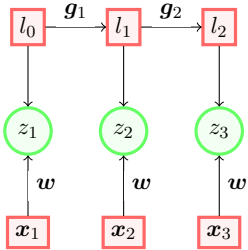

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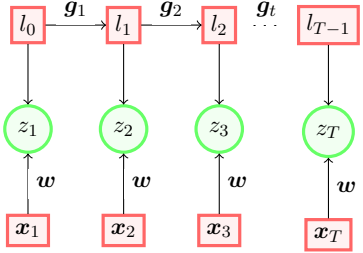

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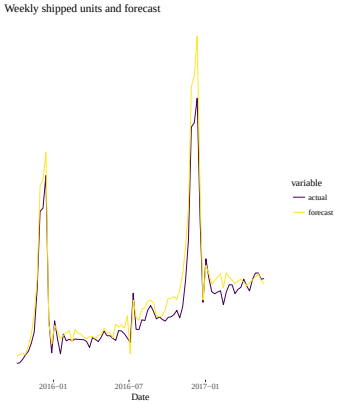
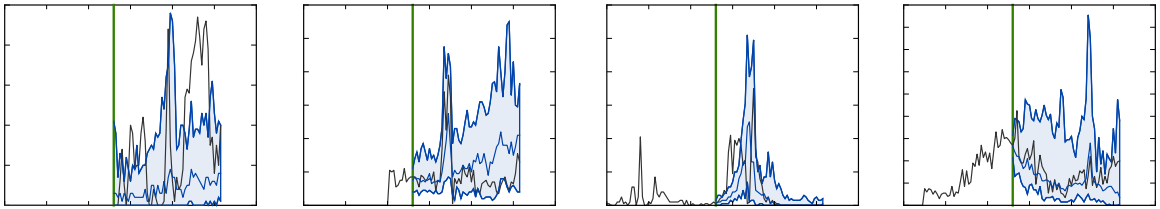
Classical methods are good for strategic forecasting problems



Predict overall Amazon retail demand years into the future.

Time series have enough history, are regular and exhibit clear patterns.

Classical models struggle with operational forecasting problems



Predict the demand for a each product available at Amazon

Time series are irregular, only combined do they have enough history and exhibit clear patterns.

The Classical Approach(es): Pros and Cons

Image (c) User:Colin / Wikimedia Commons / CC BY-SA 3.0

PROS

- De-facto standard; widely used
- Decomposition $\rightarrow$ decoupling
- White box: explicitly model-based
- Embarassingly parallel

CONS

- Requires lots manual work by experts $\Rightarrow$ hard to tune & maintain
- Cannot learn patterns across time series $\Rightarrow$ pipelines of models must be used
- Cannot handle cold-starts
- Model-based: all effects need to be explicitly modelled

Selected References

- General introduction: [Hyndman and Athanasopoulos, 2017]
- Classical textbooks: [Box et al., 2015; Brockwell and Davis, 2013]
- Exponential Smoothing and State Space Models: [Hyndman et al., 2008; Durbin and Koopman, 2012; Harvey, 1990]
- Bayesian Structure Time Series Models: [Scott and Varian, 2014; Taylor and Letham, 2018]
- Forecasting with exponential smoothing and intermittent time series: [Snyder et al., 2012]
- Approximate Bayesian inference for combination of state space and GLMs: [Seeger et al., 2016, 2017]
- Hierarchical forecasting: [Ben Taieb et al., 2017; Athanasopoulos et al., 2017; Wickramasuriya et al., 2018]
- Automatic time series forecasting: [Hyndman et al., 2007]
- ... ...

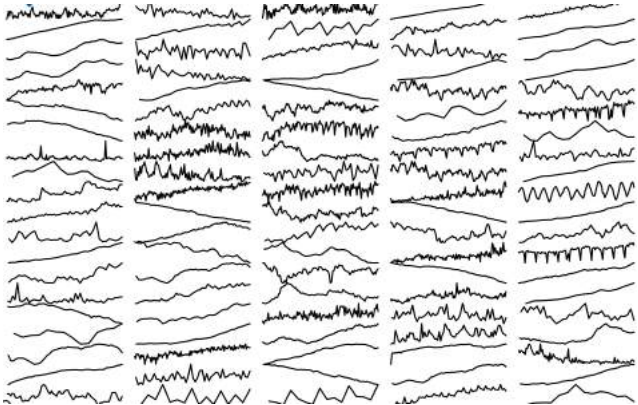
Modern Methods for Forecasting: Old and New

From Local to Global ...

- Old: local, one (preferable parsimonious!) model per time series

From Local to Global ...

- New: global, one large and complex/expressive model for all time series

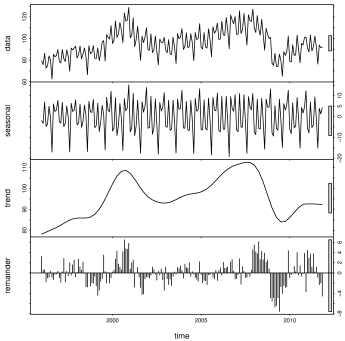


M3 Time series data visualization from [Hyndman, 2015]

Time Series Decomposition: Recap

Underlying patterns in the time series data

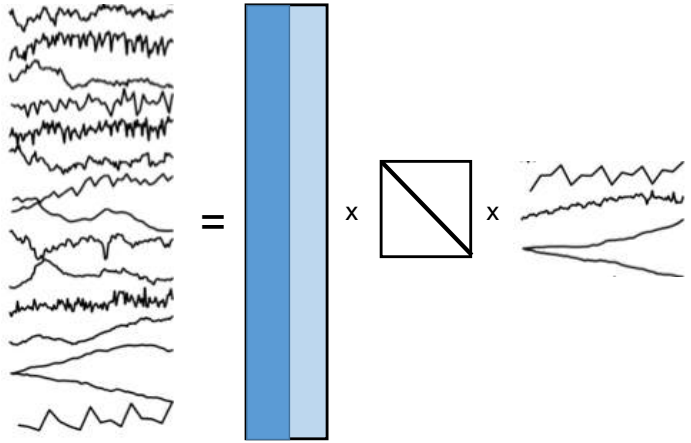
- Level
- Trend
- Seasonal variations (repeating patterns)



Questions

- How can we find common patterns across time series?
- How can we do forecast based on the learned (latent) patterns?

Matrix Decomposition

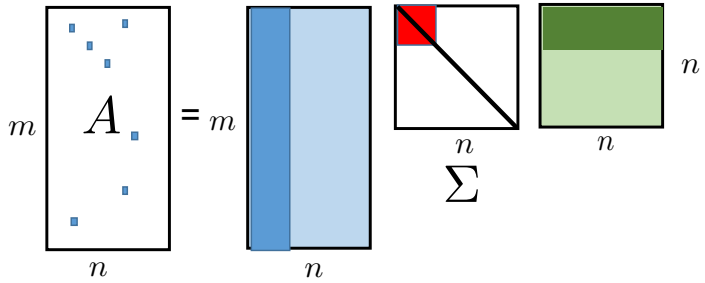


M3 Time series data visualization from [Hyndman, 2015]

Each time series is a linear combination of the hidden (time series) components.

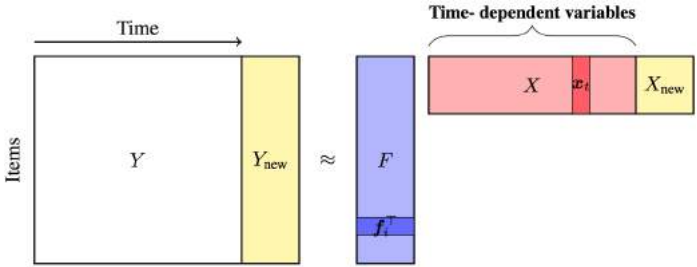
Matrix Decomposition

$$A \approx A_k = U_k \Sigma_k V_k'$$



- Perform k-SVD on the time series matrix $Z \approx U \Sigma V'$
- Use classical time series model such as ARIMA or ETS to forecast k hidden components
- Linearly combine the forecasts of the hidden components yields the individual forecasts

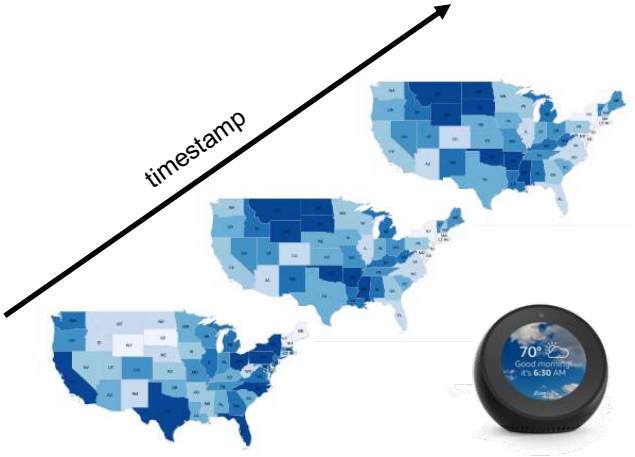
Temporal Regularized Matrix Factorization [Yu et al., 2016]



$$\min_{F,X} \sum_{(i,t)\in\Omega} (Y_{it} - \boldsymbol{f}_i^T \boldsymbol{x}_t)^2 + \lambda_f \mathcal{R}_f(F) + \lambda_x \mathcal{R}_x(X)$$

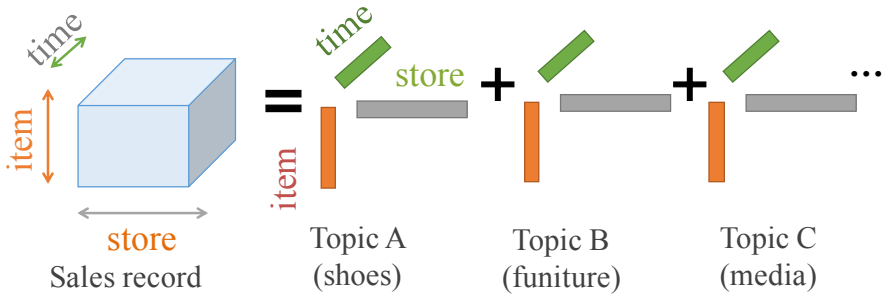
- Temporally regularization to encourage smoothness through time
- Minimizing L_2 loss without statistical assumption
- Only producing point forecasts and can not handle missing data

Tensor Decomposition: A Sample Problem



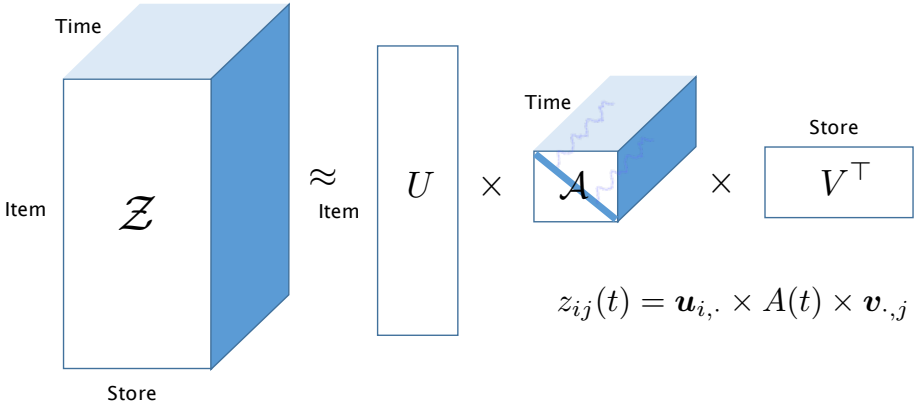
Forecast the sales for items in different locations at different time.

Tensor Decomposition: PARAFAC



Generalization of matrix decomposition for multi-view data.

Tensor Decomposition: PARAFAC



$$z_{ij}(t) = \boldsymbol{u}_{i,\cdot} \times A(t) \times \boldsymbol{v}_{\cdot,j}$$

Generalization of matrix decomposition for multi-view data.

Selected References

- Tensor decomposition and applications [Kolda and Bader, 2009]
- Latent space model for road networks to predict time-varying traffic [Deng et al., 2016]
- Autoregressive tensor factorization for spatio-temporal predictions [Takeuchi et al., 2017]
- High-Order Temporal Correlation Model Learning for Time-Series Prediction [Jing et al., 2018]
- Parcube: Sparse parallelizable tensor decompositions [Papalexakis et al., 2012]
- Fast mining and forecasting of complex time-stamped events [Matsubara et al., 2012]
- Tensorcast: Forecasting with context using coupled tensors [de Araujo et al., 2017]
- FUNNEL: automatic mining of spatially coevolving epidemics [Matsubara et al., 2014]
- ... ...

Neural Network Forecasting: Old and New – Timeline

- 1969 Weather forecasting with adaptive linear neurons (Hu)
- 1986 Backpropagation (Rumelhart et al.)
- 1988 NNs using backpropagation applied to forecasting; positive results (Werbos)
- 199x Many authors applying mostly feed-forward models to various forecasting problem (single time series)
- 1998 Review articles: "The outcome of all of these studies has been somewhat mixed"; "While ANNs provide a great deal of promise, they also embody much uncertainty."
- 2000 M3 competition – simple methods declared the winner
- 200x Less work on NN-based forecasting methods
- 2012 AlexNet wins ImageNet competition – start of the Deep Learning revival (Krizhevsky et al.)
- 2014 Generating Sequences With RNNs (Graves); seq2seq architecture (Sutskever et al.)
- 2014– Modern deep learning techniques (RNNs, CNNs) get applied to forecasting (across time series)
- 2018 M4 competition: combination of NNs and classical techniques wins

Neural Network Forecasting: Old and New

"Consensus" in the Forecasting Community: NNs don't work!

This supports the general consensus in forecasting, that neural networks (and other highly non-linear and nonparametric methods) are not well suited to time series forecasting due to the relatively short nature of most time series. The longest series in this competition was only 126 observations long. That is simply not enough data to fit a good neural network model.

– Rob Hyndman on M-challenges, 2018

Neural Network Forecasting: Old and New

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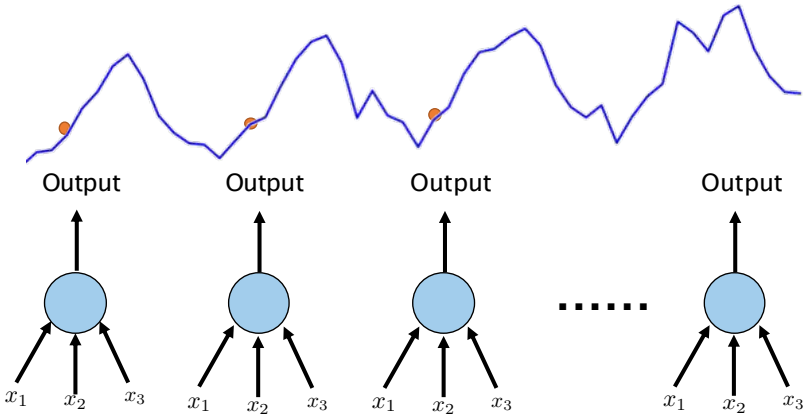
– Rob Hyndman on M-challenges, 2018

Our View

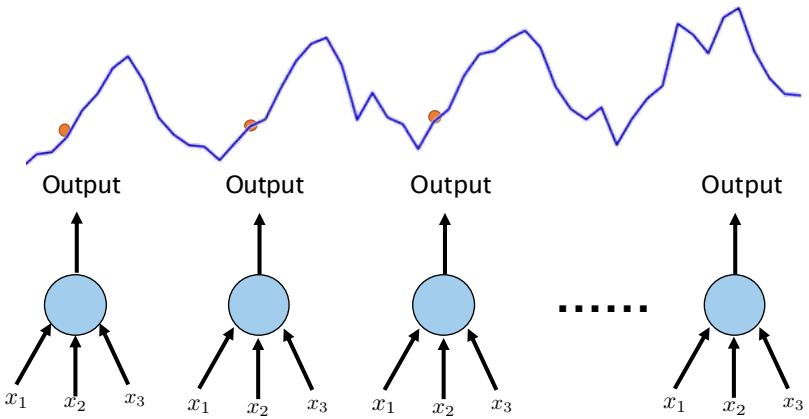
Neural networks are **great** for learning complex patterns from *many* time series in operational forecasting problems!

From Linear Regression to Feed-Forward Neural Networks



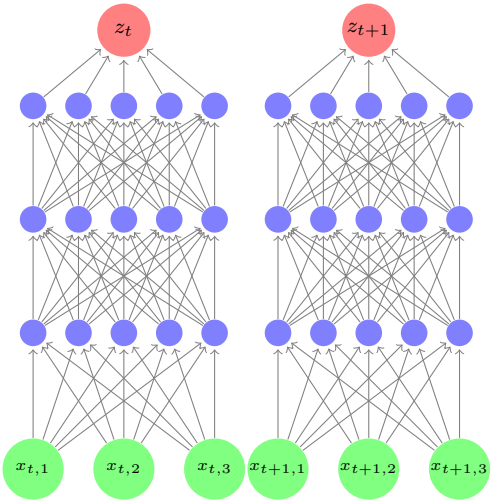
$$z_t = \boldsymbol{w}^T \boldsymbol{x}_t$$

From Linear Regression to Feed-Forward Neural Networks



$$z_t = \sigma(\boldsymbol{w}_l^T(\sigma(W_{l-1}^T(\sigma(W_{l-2}^T(\cdots W_0^T \boldsymbol{x}_t))))) := \text{DEEP-NET}(\boldsymbol{x}_t)$$

Feed-Forward Neural Networks (Multi-layer Perceptron (MLPs))

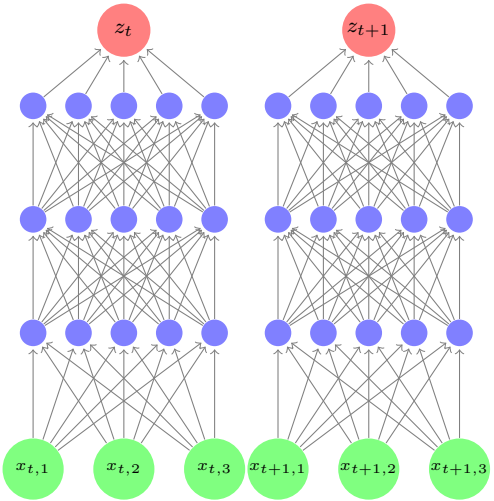


- Linear model + non-linear hidden layers
- Each neuron in a hidden layer computes an affine function of the previous layer, followed by a non-linear *activation* function,

$$h_{l,j} = \sigma\left(\mathbf{w}_{l,j}^{\top}\mathbf{h}_{l-1} + b_{l,j}\right)$$

- FF Neural Networks are flexible general function estimators
- More (and larger) hidden layers $\rightarrow$ more complex functions

Feed-Forward Neural Networks (Multi-layer Perceptron (MLPs))



- Main advantage over linear models: Can learn complex input-output relationships

$\Rightarrow$ Less manual feature engineering

- Main disadvantage: more data needed for training
- Careful tuning (e.g. of regularization, learning rate, etc.) might be necessary for good results
- Sensitive to scaling of inputs

Training Neural Networks

General recipe

Pick a class of functions $f(\mathbf{x}; \theta)$ and learn the parameters θ by minimizing some notion of error on a *training set*,

$$\theta^\star = \underset{\theta}{\operatorname{argmin}} \sum_i L\left(\mathbf{z}_i, f(\mathbf{x}_i, \theta)\right)$$

- Optimization algorithm of choice: Stochastic Gradient Descent (SGD)
  1. For each iteration $k = 1, 2, 3, \ldots$
  2. Randomly pick a *minibatch* of examples $i_1, i_2, \ldots, i_B$
  3. Compute the batch loss $L_k = \sum_b L\left(\mathbf{z}_{i_b}, f(\mathbf{x}_{i_b}, \theta)\right)$
  4. Compute the gradient of the loss $g_k = \nabla_\theta L_k(\theta)$
  5. Update the parameters $\theta_k = \theta_{k-1} - \eta g_k$
  6. (Optional but recommended: Adjust the learning rate η)

Loss Functions

- In *supervised learning*, one key modelling choice is the *loss function*.
- In the forecasting context, the loss function compares a forecast to the truth (on historical training data where the truth is known).
- For point forecasts, a loss function compares two real numbers, e.g. $\widehat{z}_t$ vs. z_t,

$$e_t = (\widehat{z}_t - z_t)^2$$

- For distribution forecasts, a loss function compares a forecast distribution F_t to a real number z_t, e.g., negative log likelihood.

Convolutional Neural Networks

- Convolutional Neural Networks (CNNs) = NNs that use *convolutional layers*
- Typical CNN model architectures combine convolutional layers with other layer types
- CNNs with 2D convolutions are extremely successful in computer vision applications

$$\Longrightarrow \text{encode spatial invariance}$$

- 1D convolutions are a promising alternative to RNNs for sequential data

$$\Longrightarrow \text{encode temporal invariance, ``stationarity''}$$

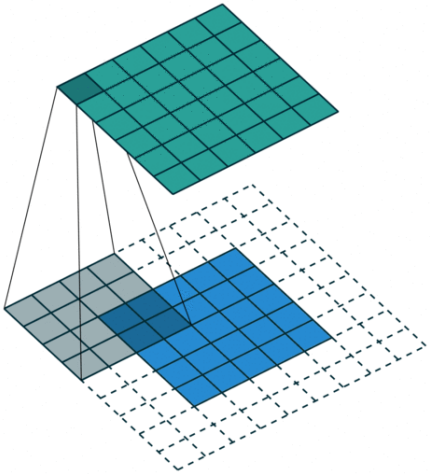
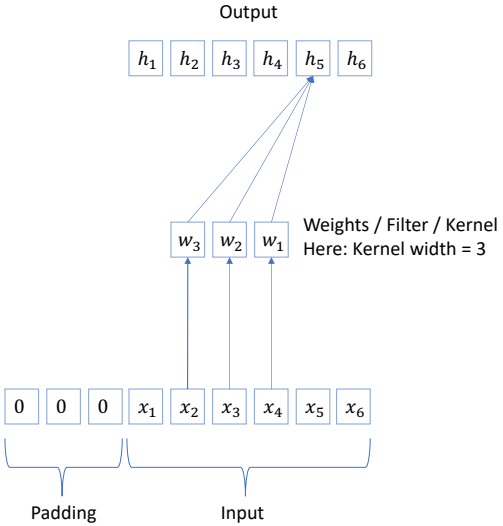


Figure credit: Vincent Dumoulin, Francesco Visin - A guide to convolution arithmetic for deep learning;
https://github.com/vdumoulin/conv_arithmetic

Convolutional Layers

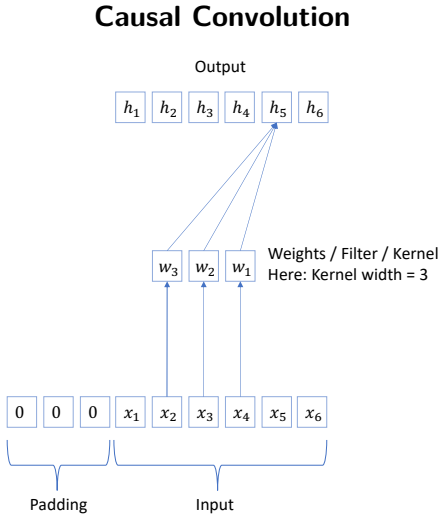


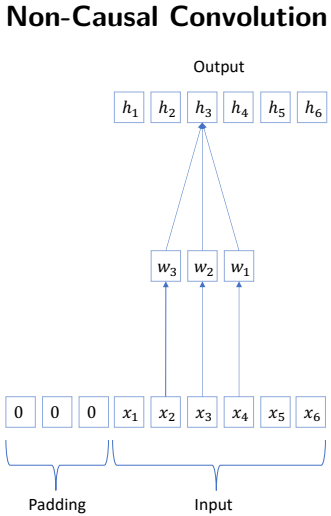
- The output h_j of a neuron j in a convolution layer is a discrete convolution of the inputs $\mathbf{x}$ with the layer's weigths/filter $\mathbf{w}$.
- For a one-dimensional convolution with a kernel with width D we have

$$h_j = \sum_{d=1}^{D} w_d x_{j-d}$$

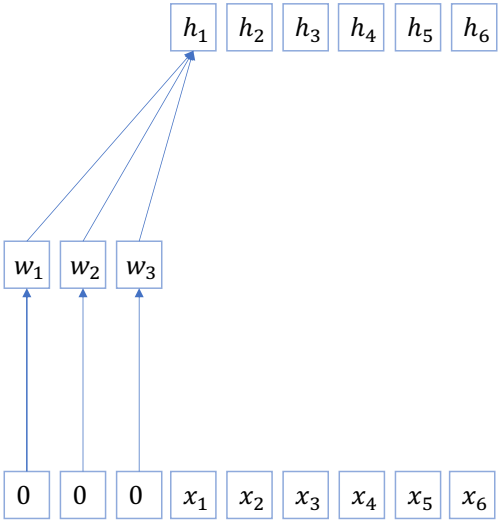
- Padding is used shift the input relative to the output and change the behavior around the edges (causal vs. non-causal)

Causal vs. Non-Causal Convolution





1D Causal Convolution



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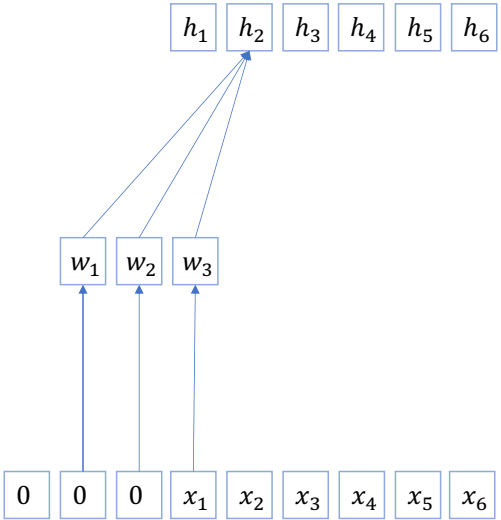

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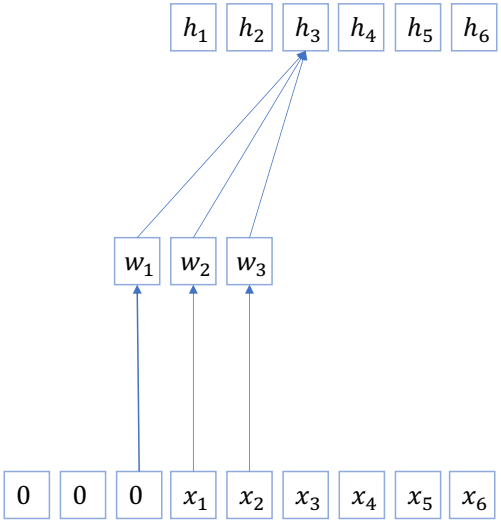

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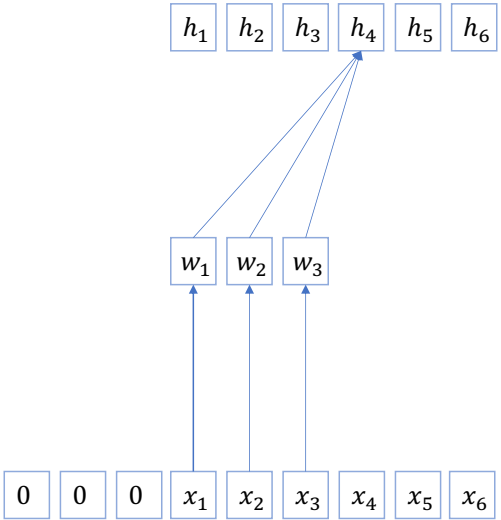

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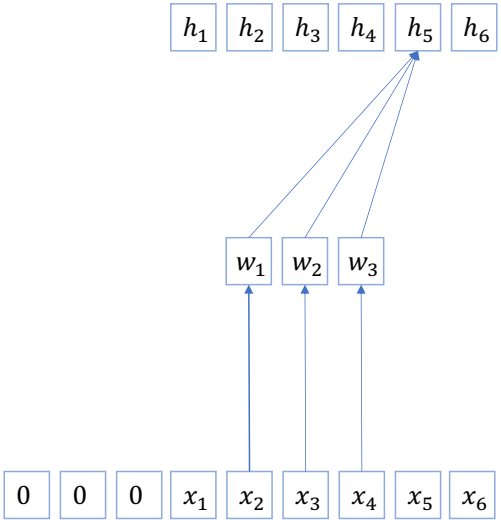

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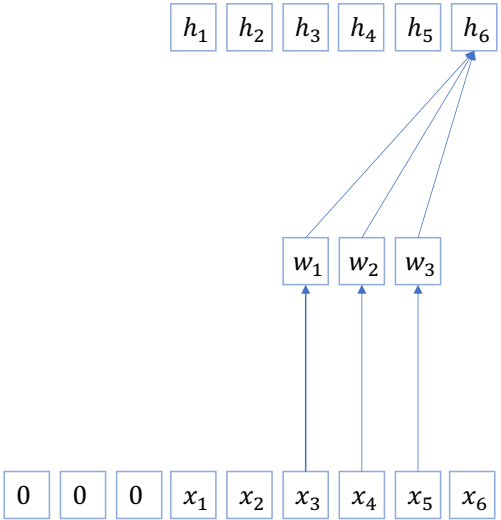
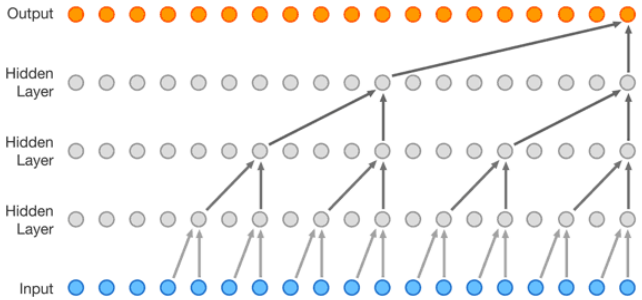


Dilated Causal Convolution and WaveNet [Van Den Oord et al., 2016]



- Dilation increases receptive field
- Forecast is generated in an autoregressive fashion
- Can be used as encoder or decoder in sequence-to-sequence (next section)
- More complex structures including gating and residual links [Van Den Oord et al., 2016]

Dilated Causal Convolution and WaveNet [Van Den Oord et al., 2016]

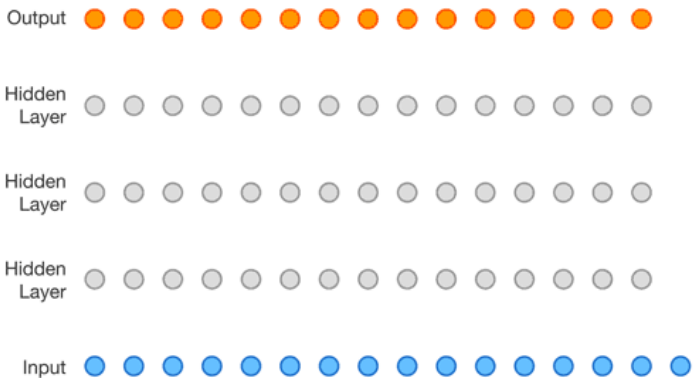
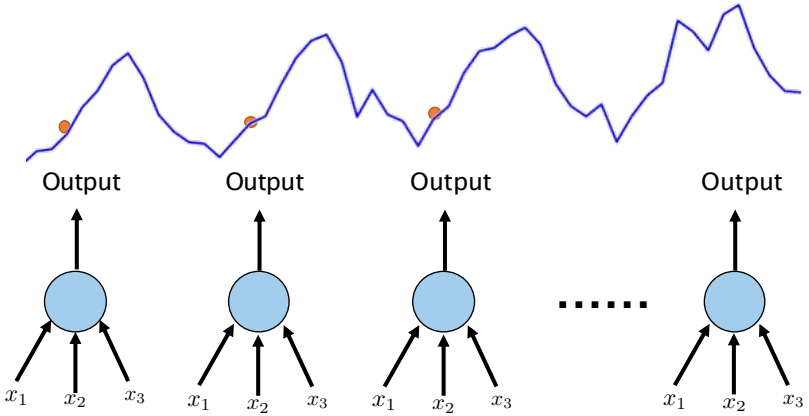


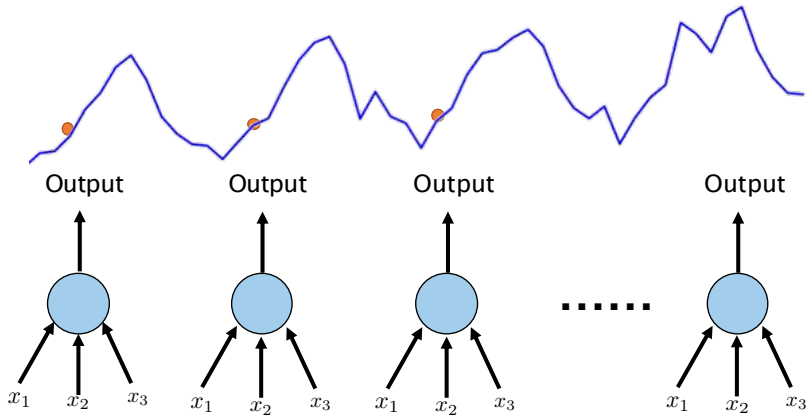
Figure credit: WaveNet: A Generative Model for Raw Audio; https://deepmind.com/blog/wavenet-generative-model-raw-audio/

Recap: MLP for Forecasting



$$z_t = \text{DEEP-NET}(\boldsymbol{x}_t)$$

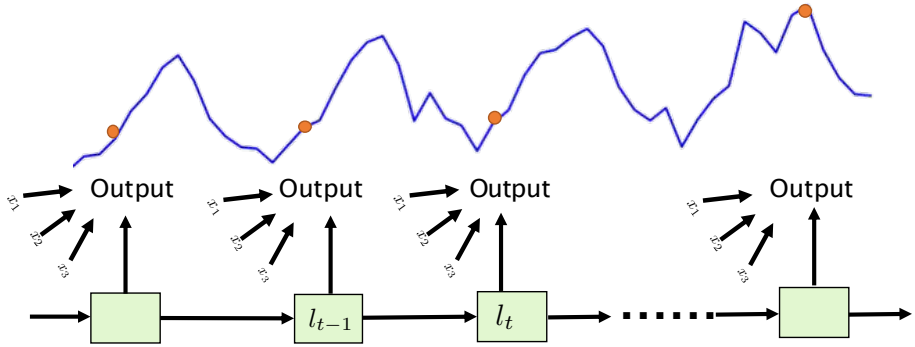
Recap: MLP for Forecasting



$$z_t = \text{DEEP-NET}(\boldsymbol{x}_t)$$

How about the sequential relationship?

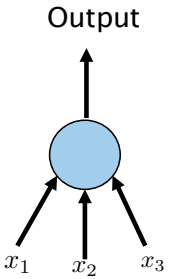
Recap: State-Space Models for Forecasting



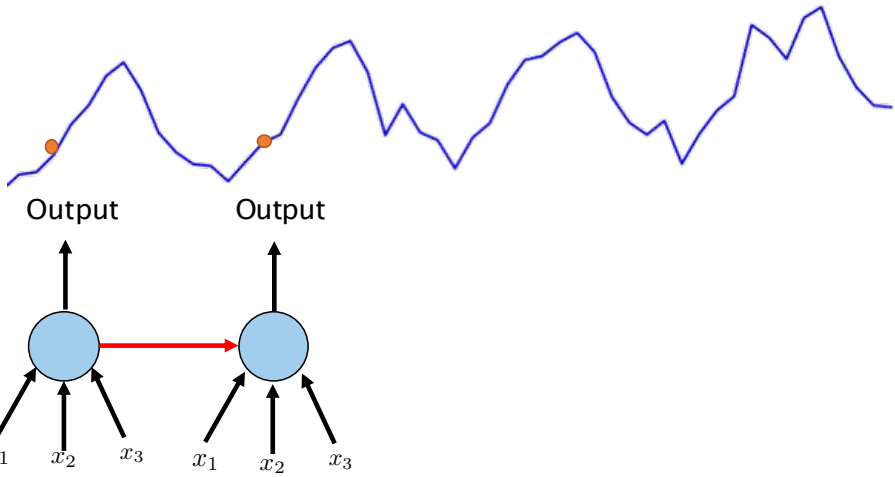
$$\boldsymbol{h}_t = \boldsymbol{l}_{t-1} + \alpha \cdot \epsilon_t$$
$$z_t = \boldsymbol{l}_t + \boldsymbol{w}^T \boldsymbol{x}_t + \epsilon_t$$

Can we do the same with NNs?

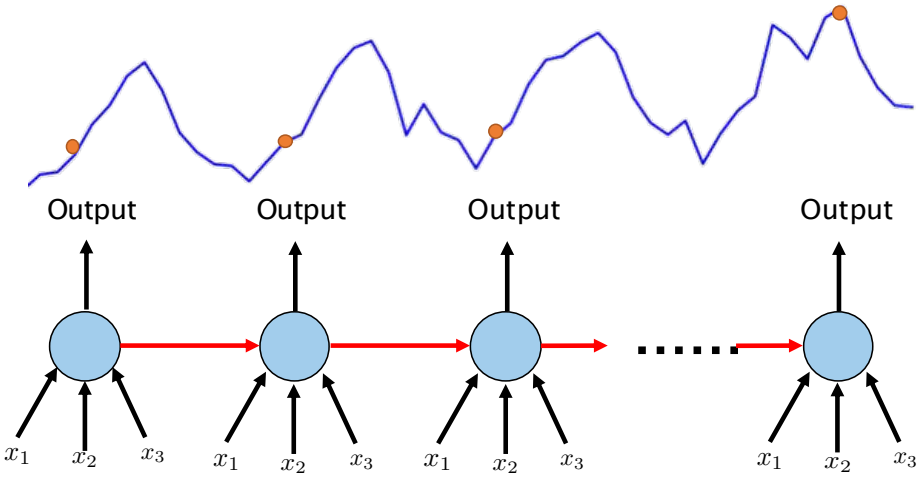
From Feed-forward NN to Recurrent NN



From Feed-forward NN to Recurrent NN



From Feed-forward NN to Recurrent NN

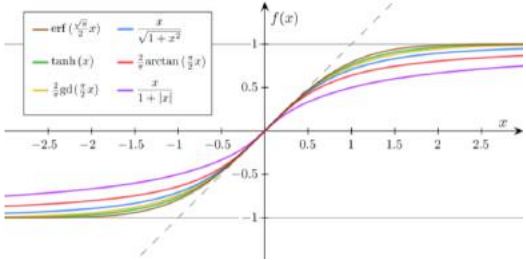


From Latent State (Exponential Smoothing) to Recurrent NN

Current hidden state h_t combines

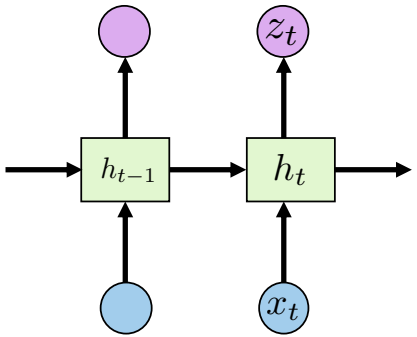
- the previous hidden state h_{t-1}
- input features x_t

and goes into



Source: Wikipedia

RECURRENT NEURAL NETWORK

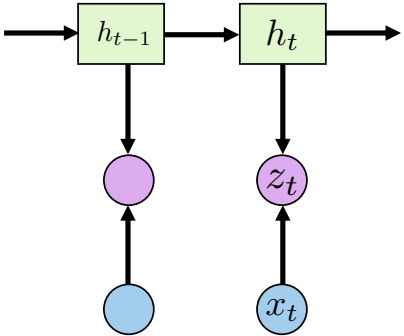


$$\boldsymbol{h}_t = \sigma(\theta_0 h_{t-1} + \theta_1 x_t)$$
$$z_t = \sigma(\theta h_t)$$

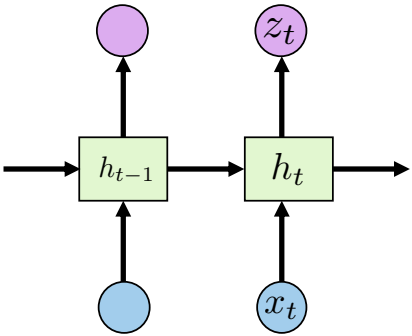
Central idea: Exponential Smoothing

today = yesterday's information + new knowledge

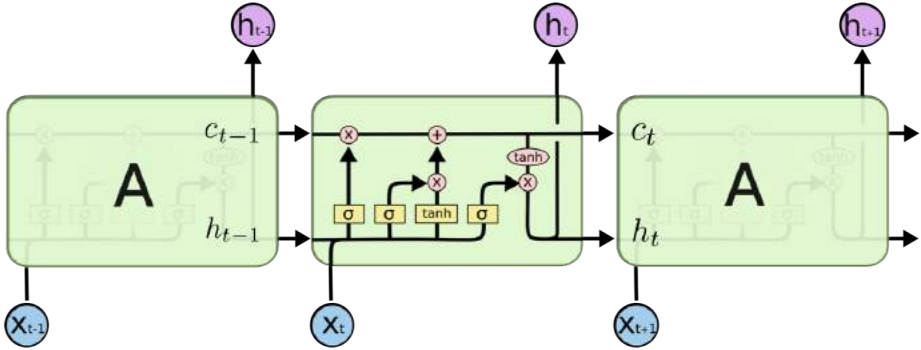
STATE-SPACE MODEL



RECURRENT NEURAL NETWORK



Long Short-Term Memory (LSTM) [Hochreiter and Schmidhuber, 1997]



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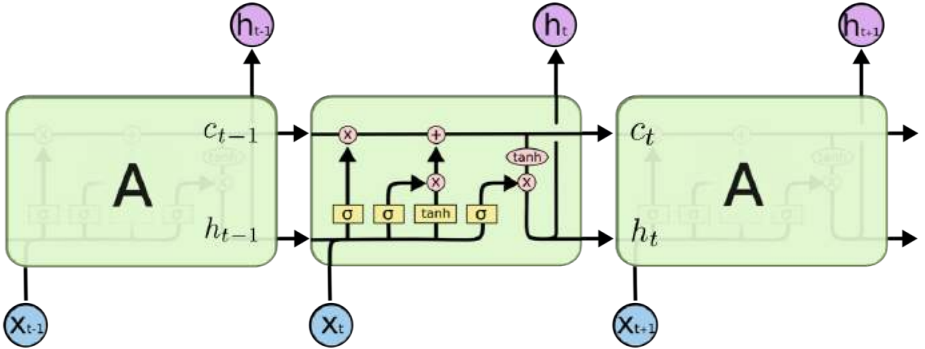
WHAT AND WHY?

Long Short-Term Memory (LSTM): What?



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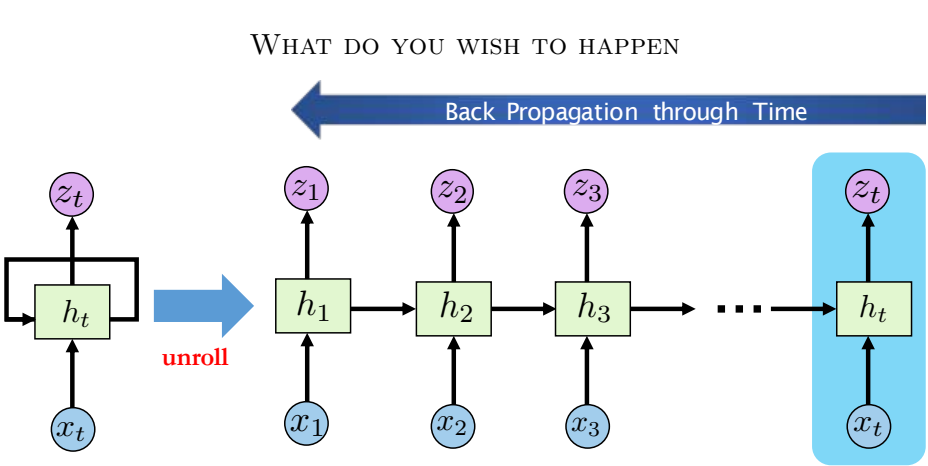
$$C_t = \alpha_t \cdot C_{t-1} + \beta_t \times \sigma(\theta_0 h_{t-1} + \theta_1 x_t)$$

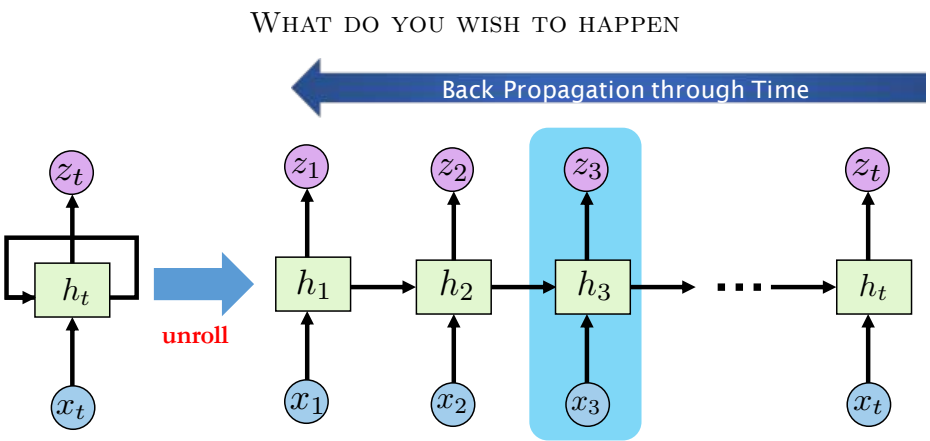
current state = forgot gate × old stuff + input gate × new stuff.

The same exponential smoothing idea!

Long Short-Term Memory (LSTM): Why?



Long Short-Term Memory (LSTM): Why?



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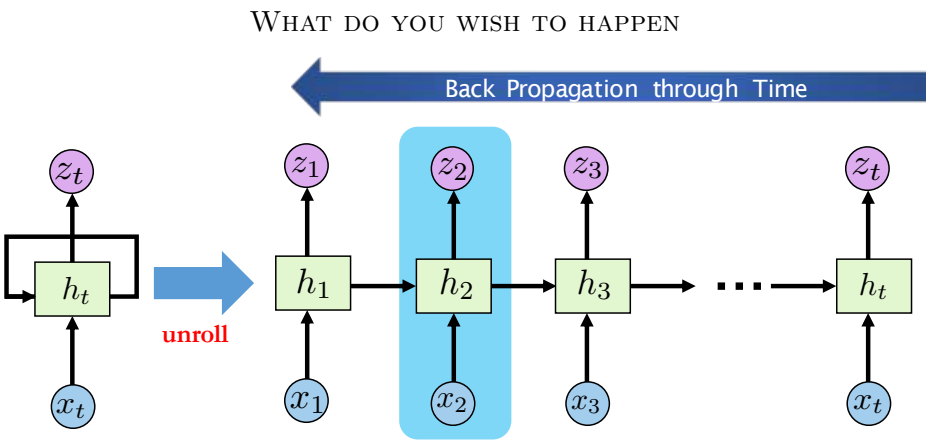
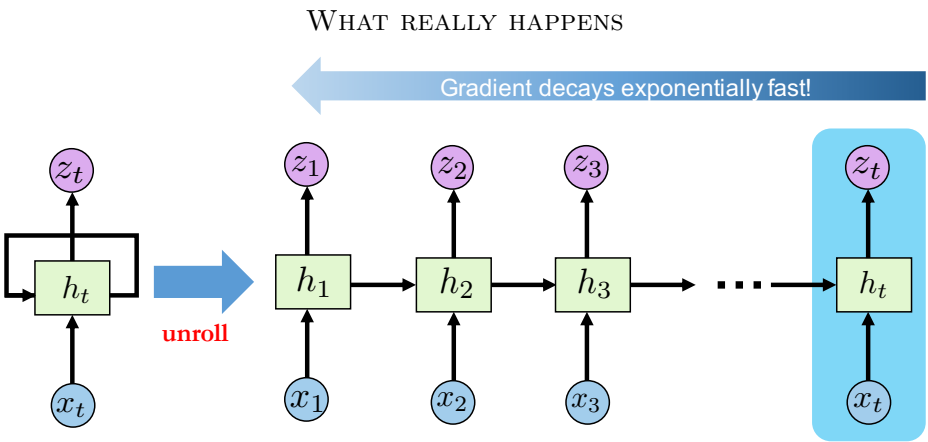
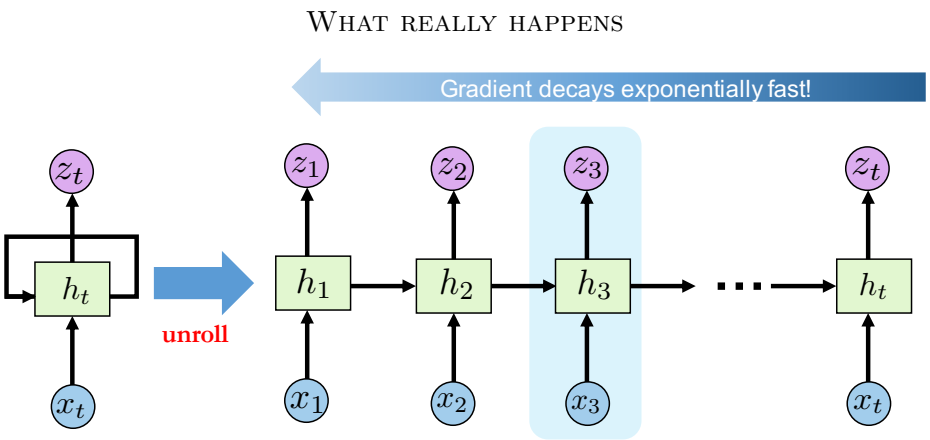


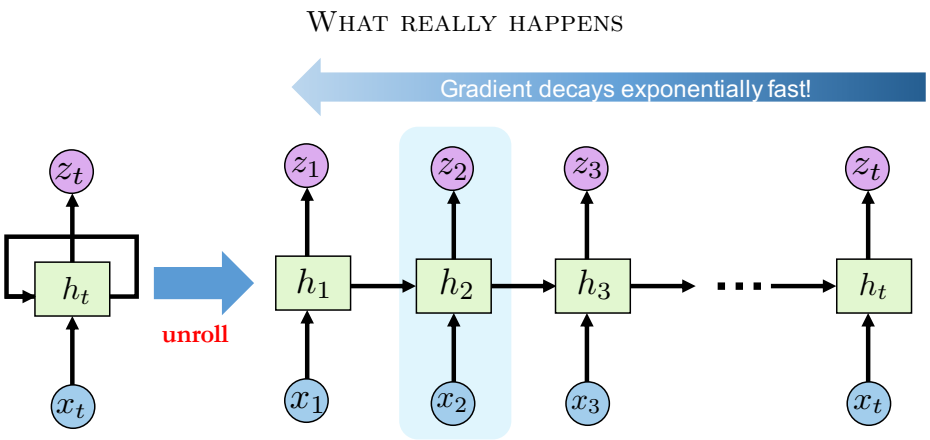
Long Short-Term Memory (LSTM): Why?



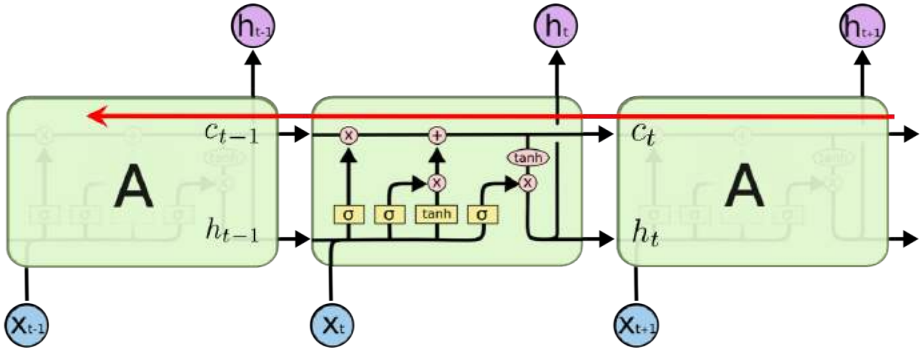
Long Short-Term Memory (LSTM): Why?



Long Short-Term Memory (LSTM): Why?



Long Short-Term Memory (LSTM): Here is Why!



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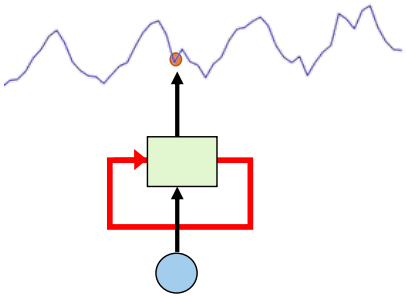
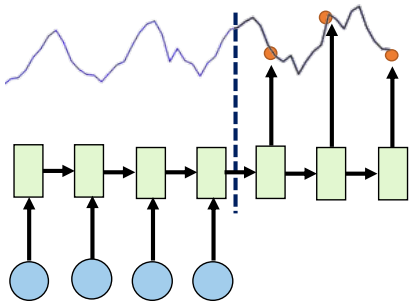
LSTM $\frac{\partial c_t}{\partial c_{t-1}} = \text{diag}(f_t)$ $c_t = f \odot c_{t-1} + i \odot g$

Canonical RNN $\frac{\partial h_t}{\partial h_{t-1}} = \theta_0$ $h_t = \sigma(\theta_0 h_{t-1} + \theta_1 x_1)$

Back to Forecasting



Canonical (One-to-One)

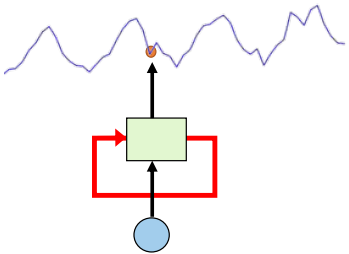


Seq2Seq (Many-to-Many)

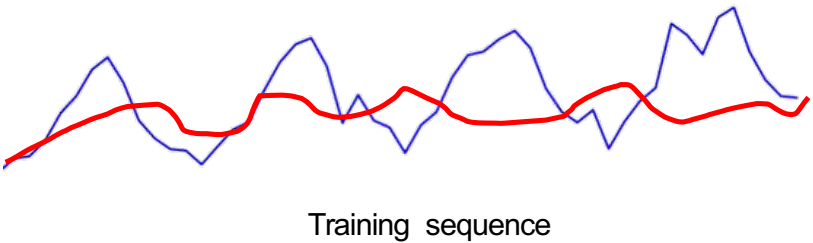
- Canonical (One-to-One) RNN: DeepAR [Flunkert et al., 2017], AR-MDN [Mukherjee et al., 2018], Deep LSTM [Yu et al., 2017a], ...
- Sequence-to-Sequence (Many-to-Many) models: Diffusion Convolutional RNNs [Li et al., 2018], MQ-RNN [Wen et al., 2017], ...

Canonical RNN Structure (One-to-One)

$$f_t : x_t \mapsto z_t$$



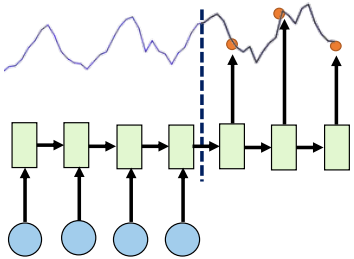
Canonical (One-to-One)



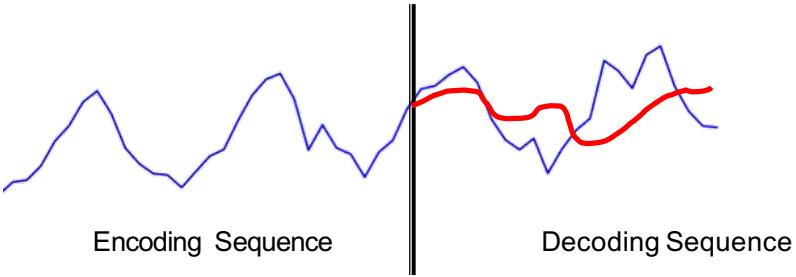
How well does the prediction reconstruct the the observed time series?

Sequence to Sequence or Seq2Seq (Many-to-Many) Structure

$$f : \{z_1, \cdots, z_{T_e}\} \mapsto \{z_{T_e+1}, \cdots, z_{T_e+T_d}\}$$



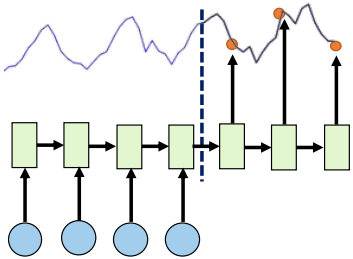
Seq2Seq (Many-to-Many)



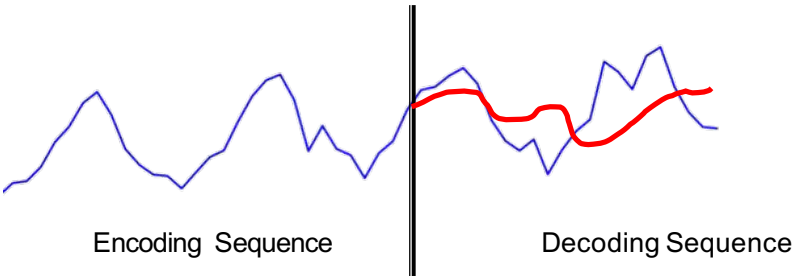
How well does the prediction reconstruct the decoding sequence conditioned on the encoding sequence?

Sequence to Sequence or Seq2Seq (Many-to-Many) Structure

$$f : \{z_1, \cdots, z_{T_e}\} \mapsto \{z_{T_e+1}, \cdots, z_{T_e+T_d}\}$$

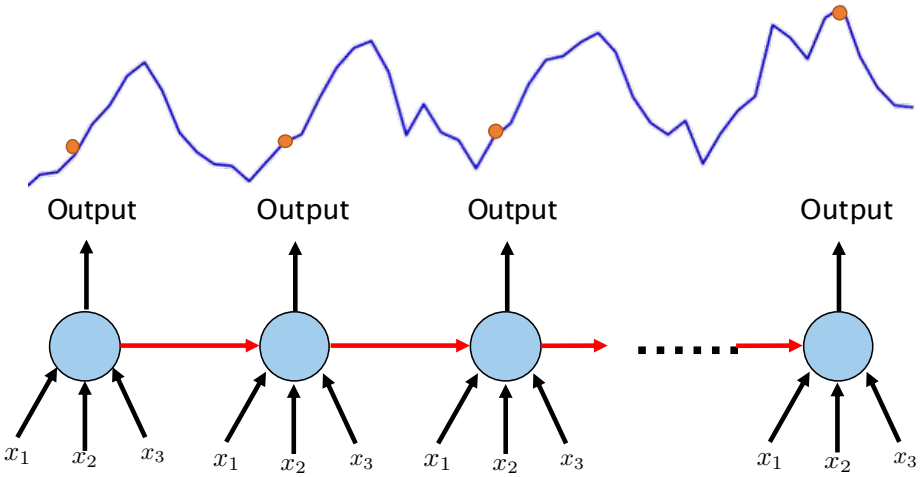


Seq2Seq (Many-to-Many)

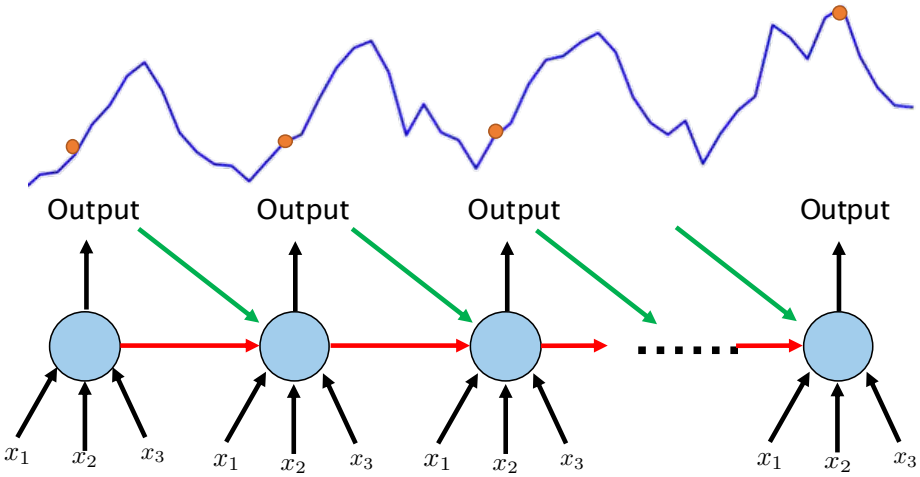


How well does the prediction reconstruct the decoding sequence conditioned on the encoding sequence? Conceptually close to multivariate regression

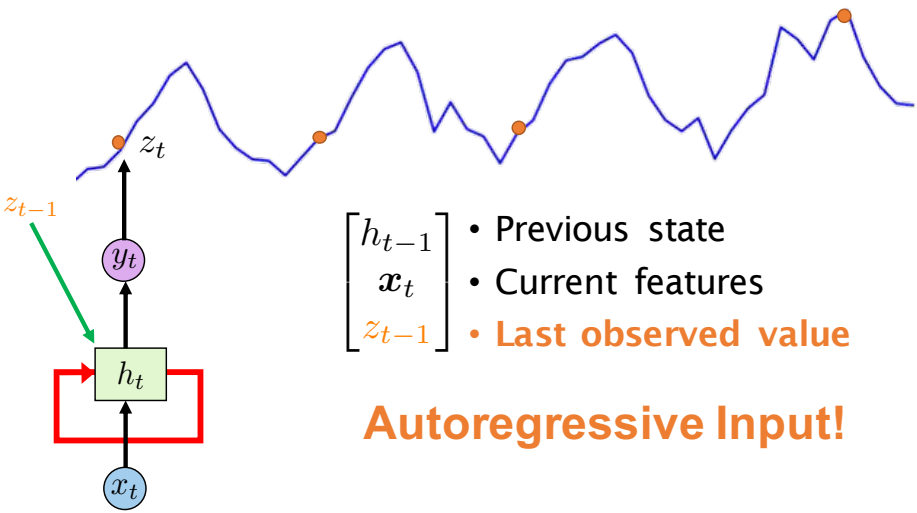
Canonical RNN Structure: DeepAR [Flunkert et al., 2017]



Canonical RNN Structure: DeepAR [Flunkert et al., 2017]



Canonical RNN Structure: DeepAR [Flunkert et al., 2017]

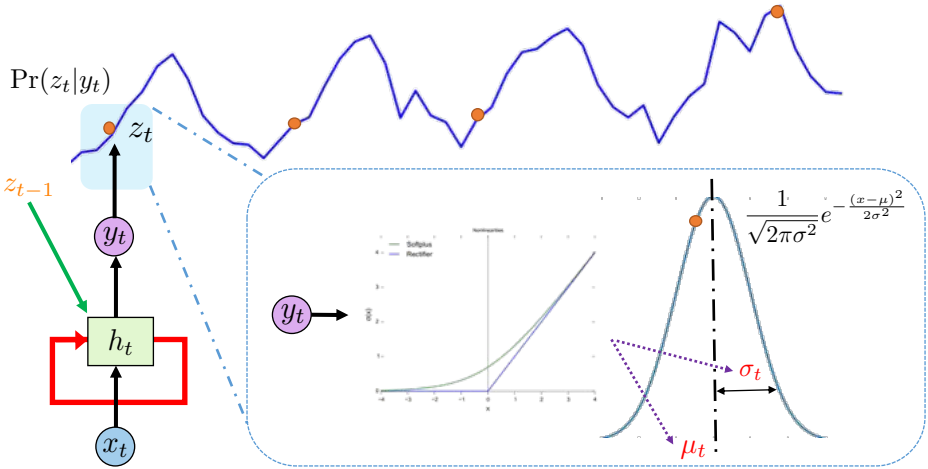


$$\begin{bmatrix} h_{t-1} \\ \boldsymbol{x}_t \\ z_{t-1} \end{bmatrix}$$

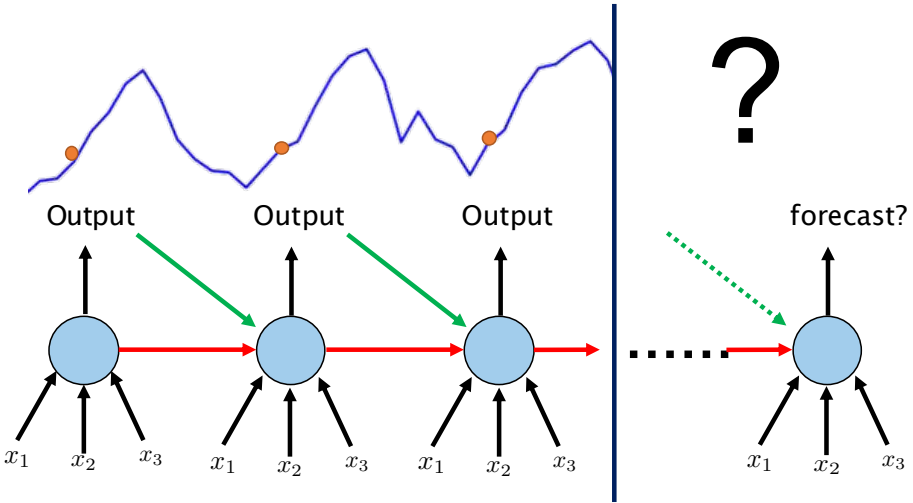
- Previous state
- Current features
- **Last observed value**

Autoregressive Input!

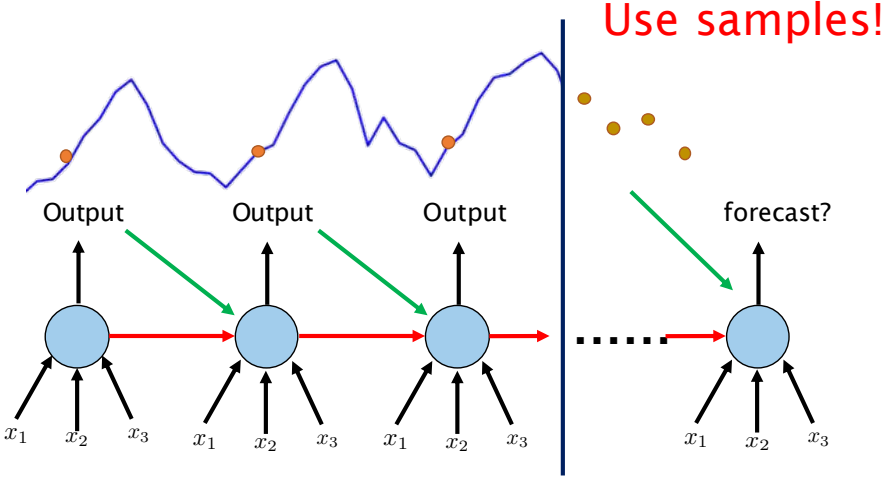
Canonical RNN Structure: DeepAR [Flunkert et al., 2017]



Canonical RNN Structure: How do we do forecast?

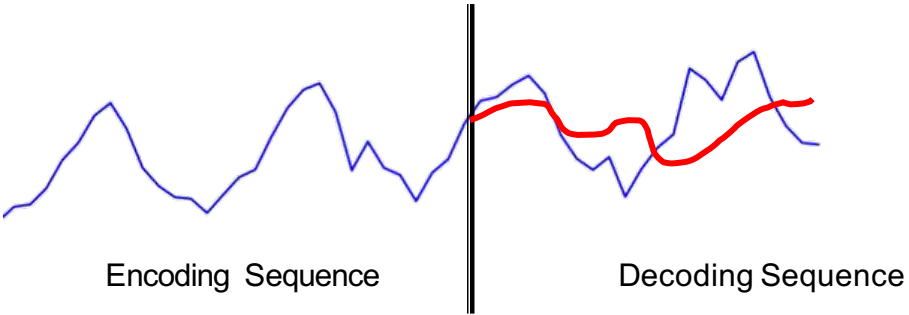


Canonical RNN Structure: How do we do forecast?

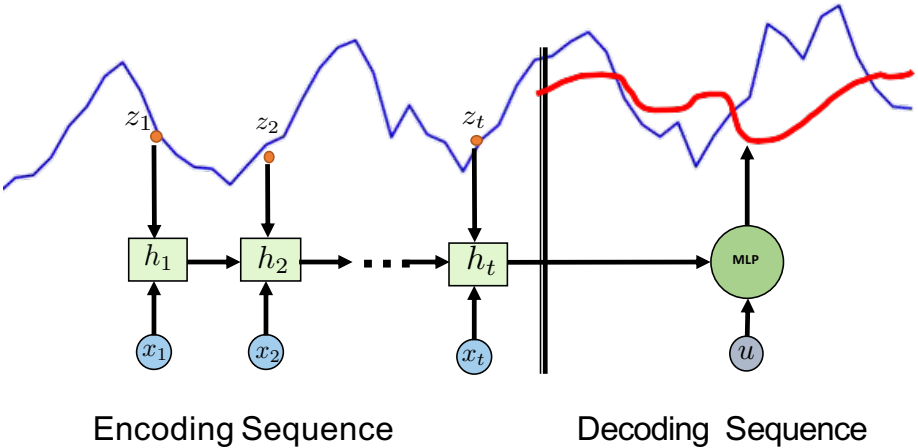


Sequence to Sequence (Seq2Seq) Structure: Many-to-Many

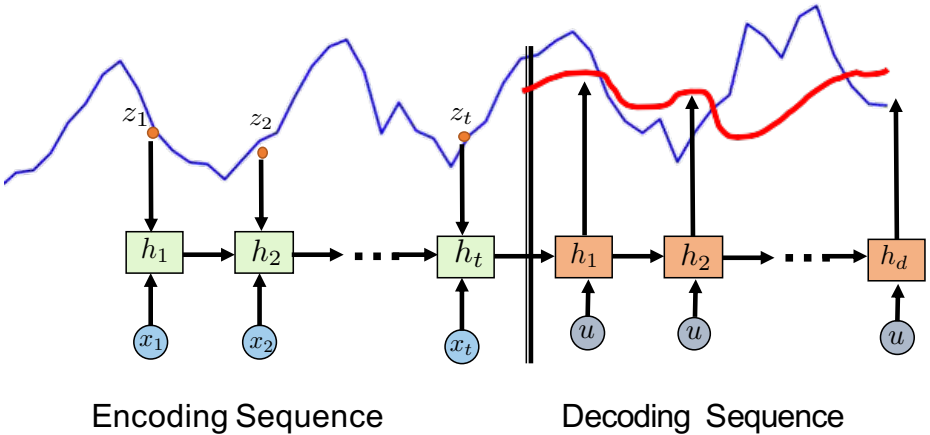
$$f_{encoder} : \{z_1, \cdots, z_{T_e}\} \mapsto \boldsymbol{h}_{T_e}$$
$$f_{decoder} : \boldsymbol{h}_{T_e} \mapsto \{z_{T_e+1}, \cdots, z_{T_e+T_d}\}$$



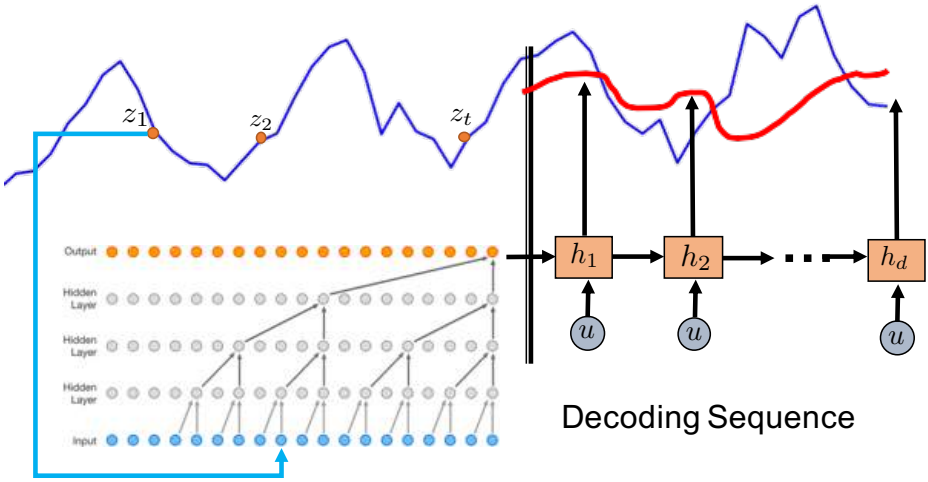
Seq2Seq: RNN-MLP [Wen et al., 2017]



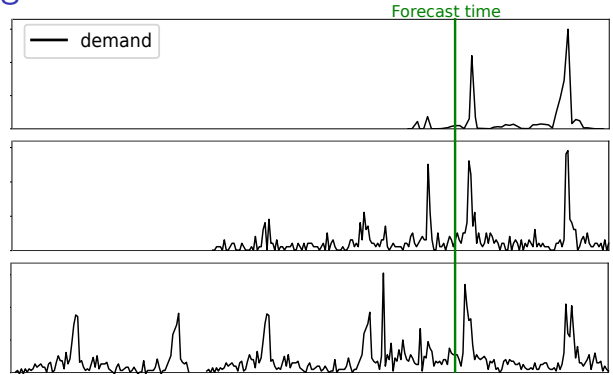
Seq2Seq: RNN-RNN



Seq2Seq: Causal CNN-RNN

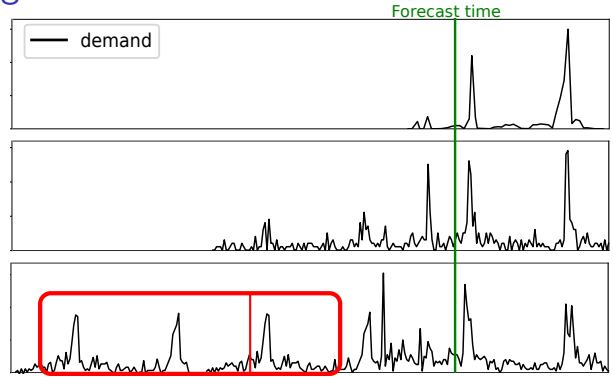


Seq2Seq: Training



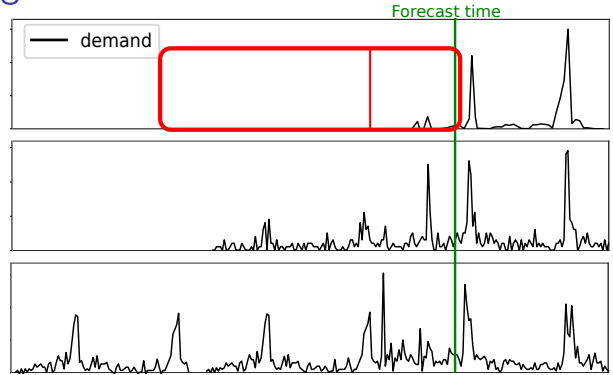
- Input:
  - time series (targets) z_t's: encoding and decoding
  - input features: encoding $\boldsymbol{x}_t$'s and decoding $\boldsymbol{u}$'s

Seq2Seq: Training



- Input:
  - time series (targets) z_t's: encoding and decoding
  - input features: encoding $\boldsymbol{x}_t$'s and decoding $\boldsymbol{u}$'s
- Slicing windows across item and time (temporal)
- Trained by minimizing certain metrics (negative loglikelihood, L_1/L_2 loss, quantile loss, etc.)

Seq2Seq: Training



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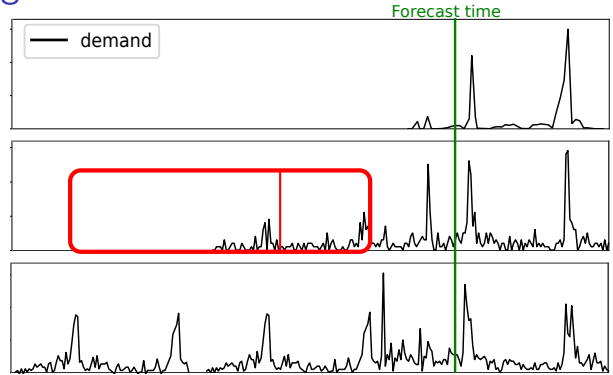
Seq2Seq: Training



- Input:
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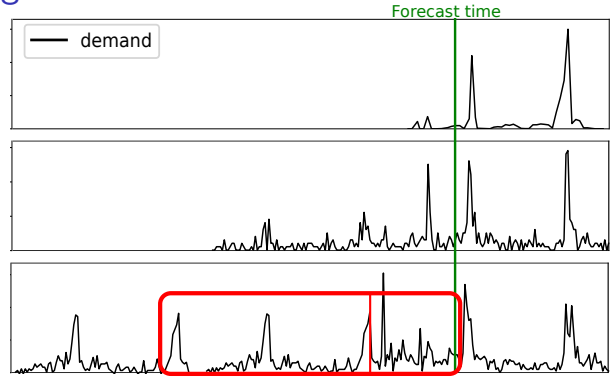
Seq2Seq: Training



- Input:
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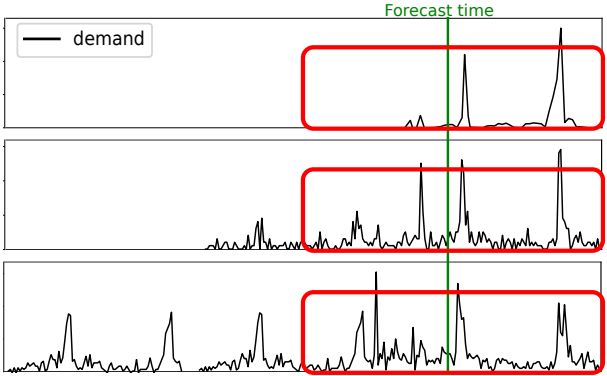
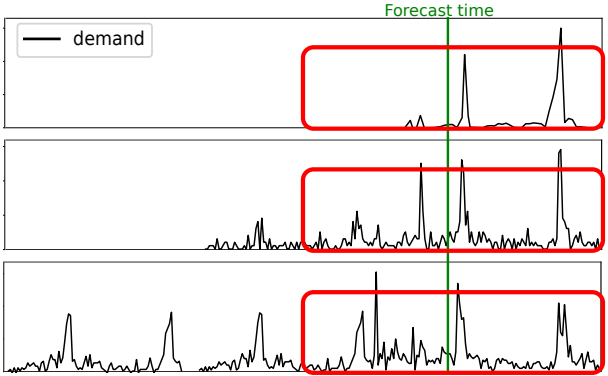
- Slicing windows across item and time (temporal)
- Trained by minimizing certain metrics (negative loglikelihood, L_1/L_2 loss, quantile loss, etc.)

Seq2Seq: Prediction

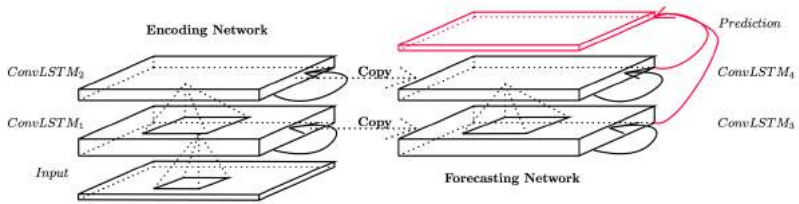


Seq2Seq: Prediction



- target z_t is unobserved after the forecast time

Seq2Seq: Convolutional LSTM [Xingjian et al., 2015]

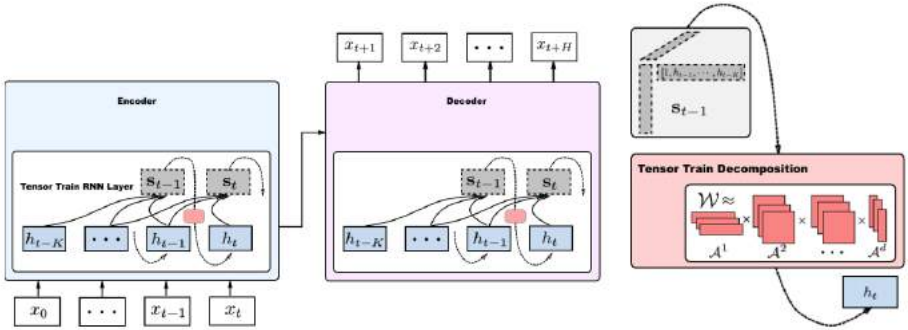


LSTM $c_t = f_t \odot c_{t-1} + i_t \odot \tanh(W_{xc} \cdot x_t + W_{hc} \cdot h_{t-1} + b_c)$

ConvLSTM $\mathcal{C}_t = f_t \odot \mathcal{C}_{t-1} + i_t \odot \tanh(W_{xc} * x_t + W_{hc} * h_{t-1} + b_c)$

- Input is time series of images (tensor data)
- Convolution happens in the spatial domain

Seq2Seq: Tensor-Train RNNs [Yu et al., 2017b]

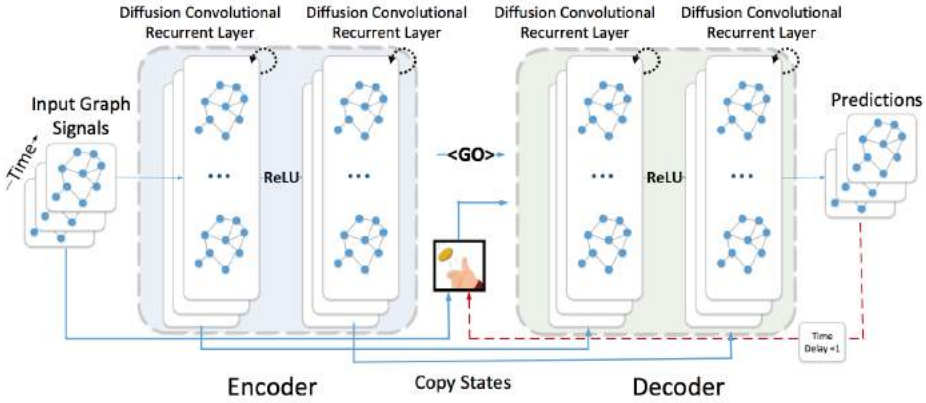


- State transition is L-th order Markov transition to capture higher-order dynamics

$$h_t = f(x_t, h_{t-1}, \cdots, h_{t-L}),$$

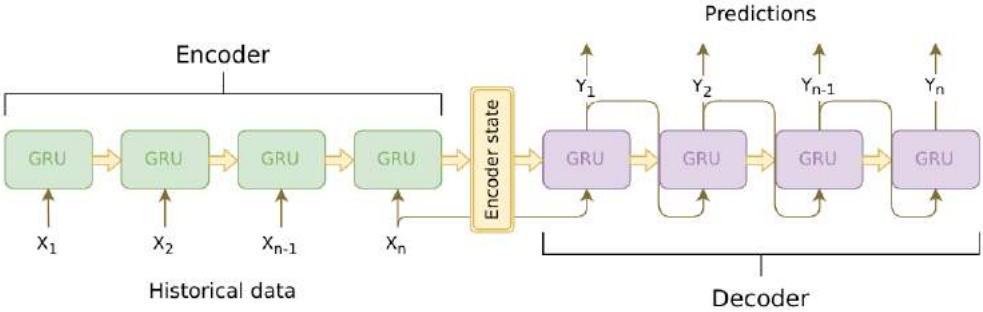
- Tensor train decomposition to approximate the weight tensor
- Polynomial interactions between the hidden states h_t and x_t

Seq2Seq: Diffusion Convolutional RNNs [Li et al., 2018]



- Pair-wise spatial correlations between traffic sensors as a directed graph
- Diffusion convolution on the graphs

Seq2Seq: Gated Recurrent Units (GRU) [Suilin, 2017]

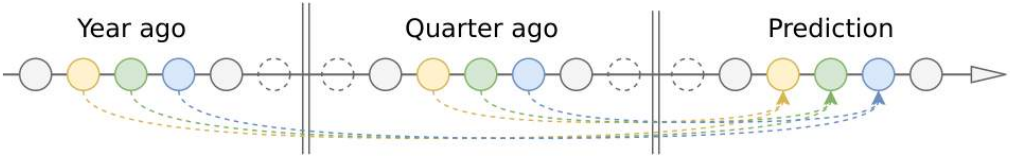


https://github.com/Arturus/kaggle-web-traffic/blob/master/how_it_works.md

- Kaggle Wikipedia winning solution: GRU and GRU decoder

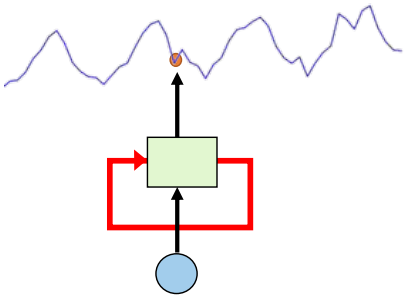
What about ATTENTION?

Lag is All You Need!

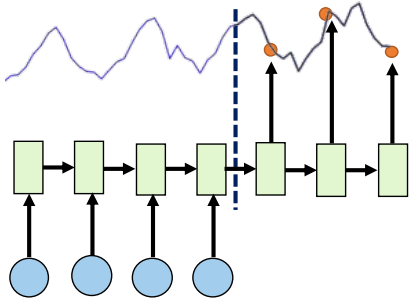


https://github.com/Arturus/kaggle-web-traffic/blob/master/how_it_works.md

Comparison: Canonical (One-to-One) vs. Seq2Seq (Many-to-Many)



Canonical (One-to-One)



Seq2Seq (Many-to-Many)

Canonical
- input features need to be available during prediction phase
- no need to re-train for different prediction length (forecast horizon)

Seq2Seq
- can have disjoint encoding and decoding features
- needs re-training when changing the decoder length

So ... Neural Networks, huh?

When to use what for which types of time series?

- MLPs are robust baseline methods, but requires heavy feature engineering
- RNNs are, the *de facto* standard model for sequence modeling. Sometimes stability problems in training.
- Recent research [Miller and Hardt, 2018; Bai et al., 2018] advocates that CNNs are as accurate but much more efficient
- But people argue that dilated RNNs [Chang et al., 2017] are just as efficient ...

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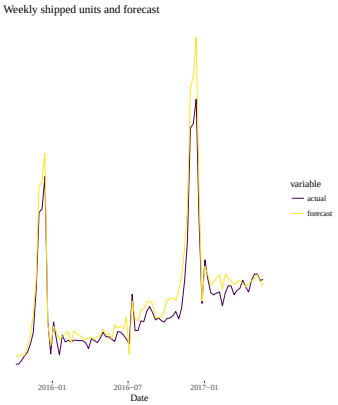
- Recent research [Miller and Hardt, 2018; Bai et al., 2018] advocates that CNNs are as accurate but much more efficient
- But people argue that dilated RNNs [Chang et al., 2017] are just as efficient ...

We do not know yet, but we will!

http://quantumfuture.net/quantum_future/homepage.htm

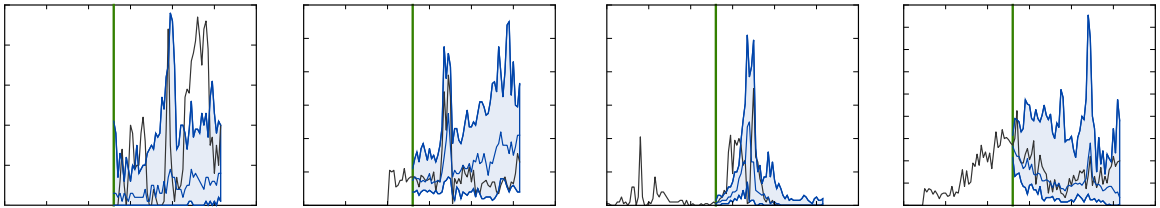
Modern methods struggle with strategic forecasting problems



Predict overall Amazon retail demand years into the future.

Not enough data may be available for training, assumptions on long-term behaviour should be handled properly. Use a classical, local model

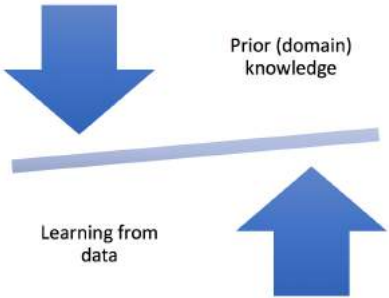
Modern models handle operational forecasting problems well



Predict the demand for a each product available at Amazon

Time series are irregular, only combined to they have enough history and exhibit clear patterns.

Finding the right balance: data vs model driven

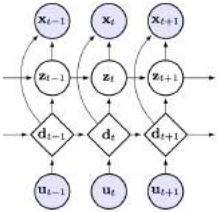
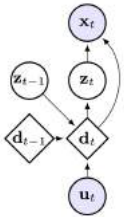
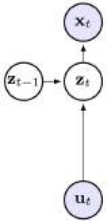
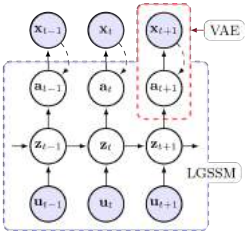


Goals:

- increase data efficiency: data efficiency improves sample complexity
- improve interpretability: interpretability facilitates better decision-making
- enforce structure: structure enables fast computation

Combining Probabilistic Graphical Models (PGM) and DNN

Efficient inference of PGM with the flexibility and expressibility of DNN

SRNN [Fraccaro et al., 2016]	VRNN/SSL/LSTM-LDA [Chung et al., 2015; Zaheer et al., 2017; Zheng et al., 2017]	DMM [Krishnan et al., 2017, 2015]	KVAE/DVBF [Fraccaro et al., 2017; Karl et al., 2017]
			

Further avenues: hybrid global-local models.

Selected References

- NN Forecasting in the early days: [Tang et al., 1991; Azoff, 1994; Gately, 1995; Zhang et al., 1998]
- Convolution structure for sequence modeling: [Van Den Oord et al., 2016; Bai et al., 2018]
- Deep Forecast: Deep Learning-based Spatio-Temporal Forecasting [Ghaderi et al., 2017]
- Autoregressive Convolutional Neural Networks for Asynchronous Time Series [Bińkowski et al., 2017]
- Improving Factor-Based Quantitative Investing by Forecasting Company Fundamentals [Alberg and Lipton, 2017]
- Time-series extreme event forecasting with neural networks at Uber [Laptev et al., 2017]
- An overview and comparative analysis of recurrent neural networks for short term load forecasting [Bianchi et al., 2017]
- ... ...

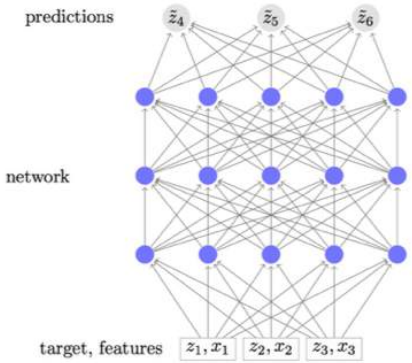
Building Forecasting Systems: Old and New

Pecularities of forecasting systems

- Time plays a role: important for backtesting & evaluation
- main primitive type are time series (one dimension more than usual)
- difference between data at train and inference time
- long feedback cycles (e.g., compare with recommender systems)
- complex interaction with downstream decision problems
- traditionally batch system, moving towards on-demand/real-time systems
- B2B not B2C scenario
- users are typically Business Intelligence officers, analysts, data scientists or business functions

Forecasting Systems: Two Extremes

vs

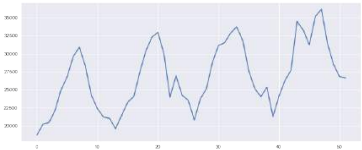


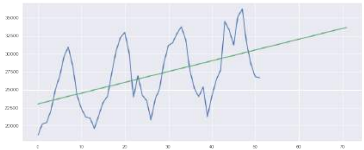
A complex pipeline of simple model vs. a complex model in a simple pipeline.

Example: m4 forecasting competition. Won by neural network approach, follow-up by ensemble methods. [Makridakis et al., 2018]

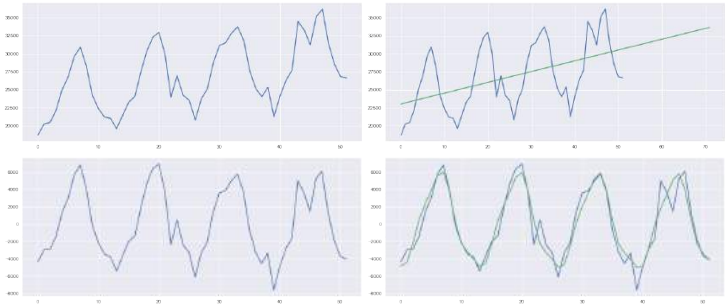
Building Forecasting Systems with Classical Models

Building Forecasting Systems with Classical Models

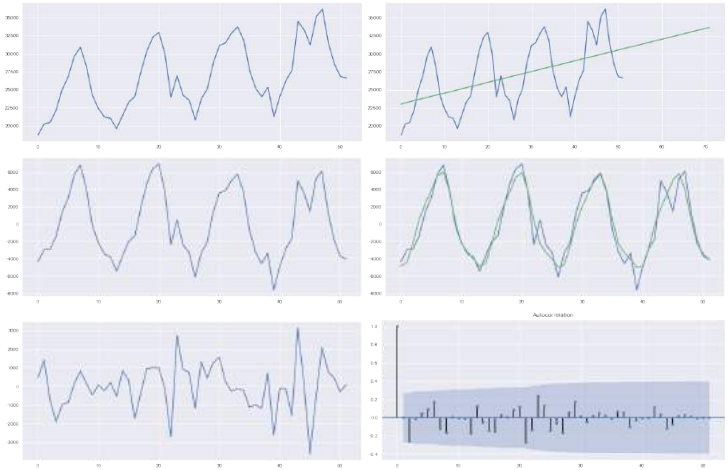




Building Forecasting Systems with Classical Models



Building Forecasting Systems with Classical Models



Forecasting Systems with classical models

Image (c) User:Colin / Wikimedia Commons / CC BY-SA 3.0

PROS

- models are canonical and relatively easy to understand
- Decomposition $\rightarrow$ decoupling
- White box: explicitly model-based
- Embarassingly parallel

CONS

- Requires lots manual work by experts $\Rightarrow$ hard to tune & maintain
- Cannot learn patterns across time series $\Rightarrow$ pipelines of models must be used
- Cannot handle cold-starts
- Model-based: all effects need to be explicitly modelled

Notable Non-Advantages

interpretability even though each model may be interpretable, the pipeline is not.

running time even though each models runs quickly, entire pipeline does not $\rightarrow$ on-demand forecasting hard to realize.

simple infrastructure forecasting pipeline require complex model combination mechanisms and feature preprocessing.

further things maintainability, tunability, ...

Forecasting System Architecture

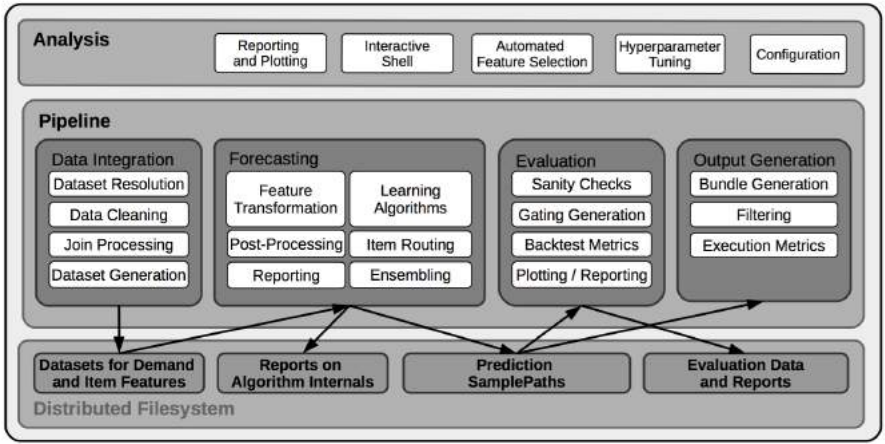
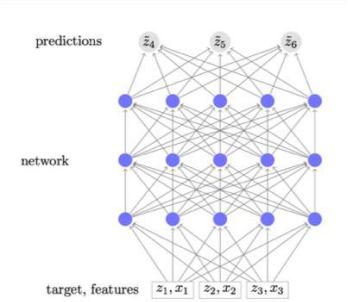


Figure from *Probabilistic Demand Forecasting at Scale* [Böse et al., 2017]

Neural Forecasting Approaches



PROS

- litte feature engineering needed
- learns across time series
- quick at inference
- default settings lead to surprinsingly good results
- state-of-the art performance in competitions

CONS

- little control over predictions
- potentially high-variance in training
- costly to train
- model serving infrastructure needed

Recent public competitions won by neural forecasting approaches: m4 competiton, wikipedia Kaggle competition.

Third Prinicple

Conservation law

Forecasting systems are complex.

Classical forecasting system

Neural forecasting system

Naturally, combinations of both extremes are possible.

Forecasting system are ML systems

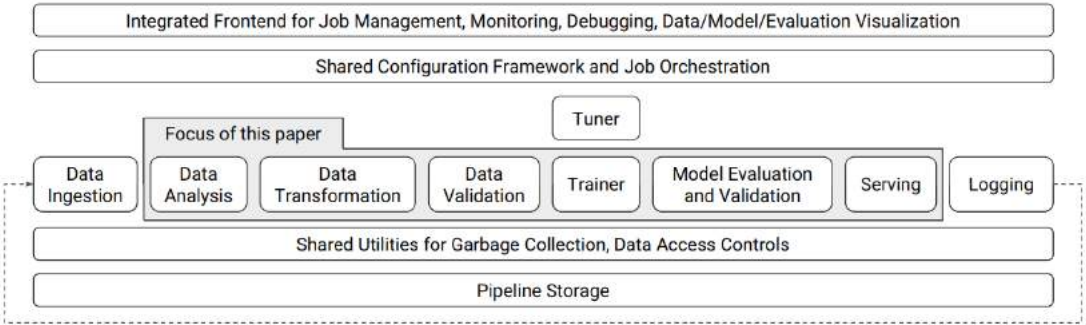


Figure from [Polyzotis et al., 2017]

ML systems: uncomprehensive laundry list of components

- ETL & Data Provenance management
- Data Cleaning, Imputation & monitoring (both for training and inference data)
- feature transformation component
- model training & experiment tracking
- model ensembling
- hyper-parameter optimization & Auto-ML/Meta-Learning
- model serving & management
- model monitoring
- live testing: bandits & A/B tests
- reporting & plotting & notebook
- configuration & orchestration
- ...

Take away: many challenges. See more in [Modi et al., 2017].

Selected References

- TFX: [Modi et al., 2017; Polyzotis et al., 2017]
- Spark-based ML: [Boehm et al., 2016; Meng et al., 2016; Sparks et al., 2017]
- Declarative ML: [Schelter et al., 2016]
- Data verification: [Schelter et al., 2018]
- Missing data: [Biessmann et al., 2018]
- Model serving: [Crankshaw et al., 2017, 2015]
- Experiment and Meta-Data Tracking: [Schelter et al., 2017]

Selected References: Forecasting competitions

M4 competition: [Makridakis et al., 2018] (and predecessors)

- Winning entry: https://eng.uber.com/m4-forecasting-competition/

Kaggle competitions on forecasting:

- Rossmann store sales: https://www.kaggle.com/c/rossmann-store-sales
- Wikipedia traffic forecast: https://www.kaggle.com/c/web-traffic-time-series-forecasting

Getting Started with Forecasting

Open-source forecasting packages: Classical methods

Rob Hyndman's R package [Hyndman et al., 2007] is among the most popular packages. Contains implementations for many classic methods. Very robust, very hard to beat. You have to like R.

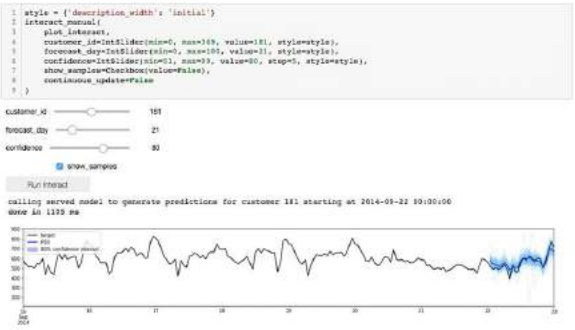
PROPHET

Facebook's Prophet package [Taylor and Letham, 2018] uses Stan [Carpenter et al., 2017] behind the scences. Very flexible but the inference is slow.

Open-source deep forecasting packages

MXNet/Gluon [Chen et al., 2015] contains a number of notebooks (linked from our website) to get started, e.g., https://gluon.mxnet.io/chapter12_time-series/lds-scratch.html

Forecasting Software: AWS SageMaker



Visit our booth for the DeepAR Demo!

THANK YOU FOR ATTENDING!




Website: https://lovvge.github.io/Forecasting-Tutorial-VLDB-2018/

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