TIME-SERIES ANALYSIS & DEEP-LEARNING

June 17^{th}, 2022

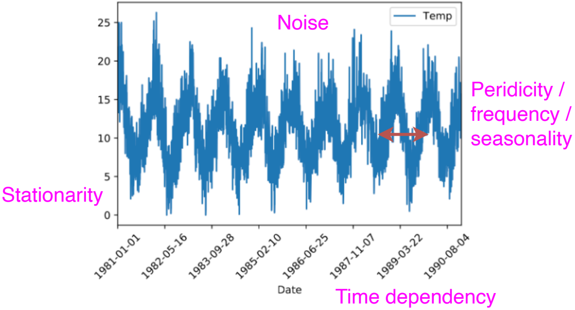
Vincent Guigue

Introduction

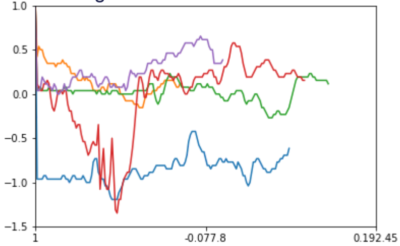
General schedule

1. Signal specificities
2. Very different applications
3. Different points of view
4. Benefits/pitfalls of ML approaches
5. Benefits of deep learning

Single instance



Variable length



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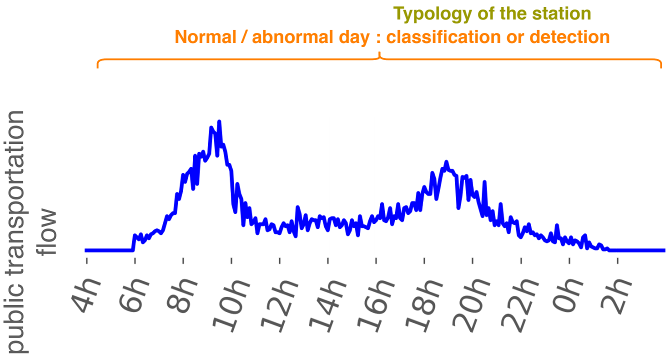

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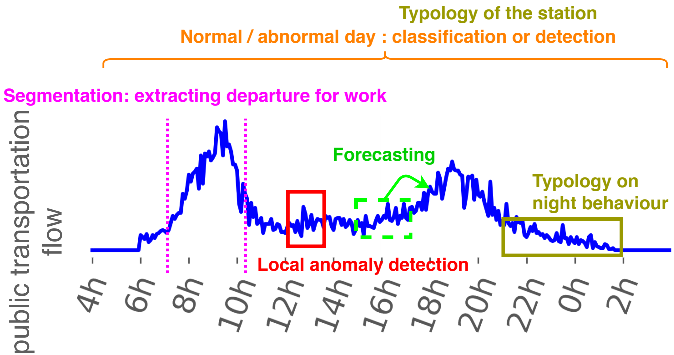

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Data Science

Statistics

Computer Science

Sales history

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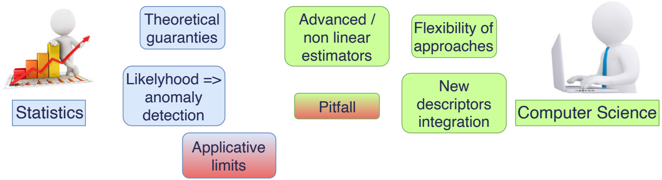

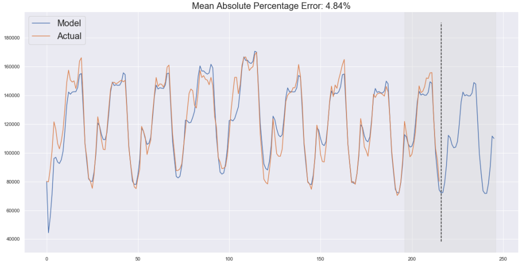

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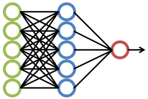
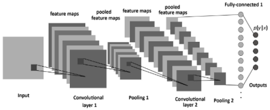
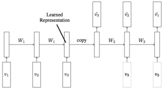
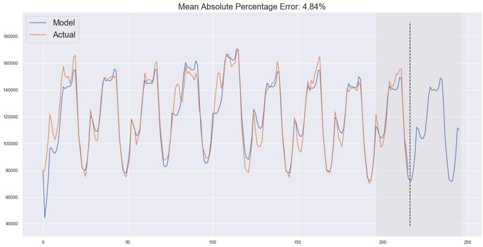
Which architecture for which application ?
... And which benefits ?



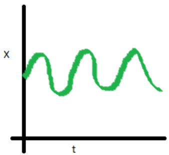




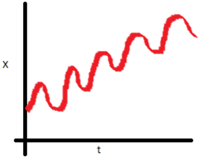


Time series = specific object

- Variable length
  - An issue... Or not
- Noise & de-noising
  - Specific de-noising strategy based on temporal dependency
- Stationarity / Periodicity
  - Constant statistical properties over time (mean, std. dev.)

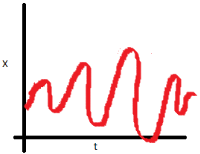


Stationary series



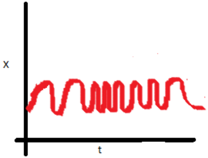
Non-Stationary series

Variable mean



Non-Stationary series

Variable std. dev.



Non-Stationary series

Variable covariance

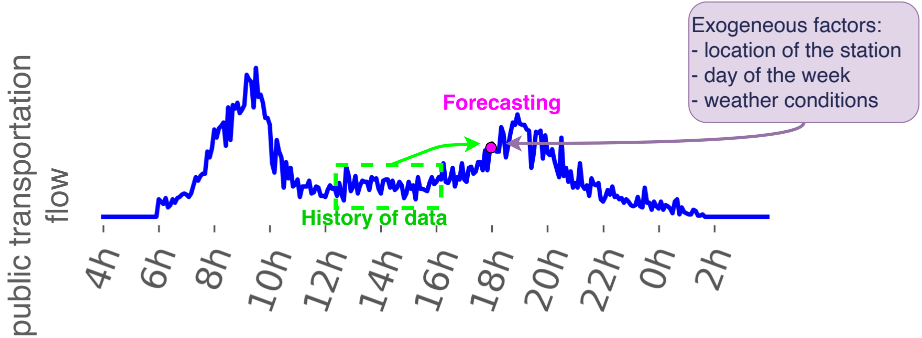
- Number of instances
  - May be one !

Statistical forecasting of next values

Forecasting task

1. Modeling prediction from history only
2. Adding context = exogenous factors

> Prediction is very difficult, especially about the future
>
> *Niels Bohr*



Can be applied on single/multiple instance problem.

Auto-Regressive approaches

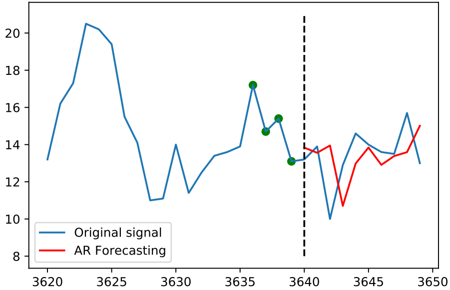
AR/ARMA

The historical answer to time-series forecasting (from statiticians)

AR : Auto-Regressive modeling :

$$Y_t = \alpha + \alpha_1 Y_{t-1} + \alpha_2 Y_{t-2} + \ldots + \alpha_p Y_{t-p} + \varepsilon_1 \quad (1)$$

Complete Guide to Time Series Forecasting in Python, https://www.machinelearningplus.com/time-series/arima-model-time-series-forecasting-python/



AR (order 4) : 4 last measures are weighted by α to predict T

Auto-Regressive approaches

AR/ARMA

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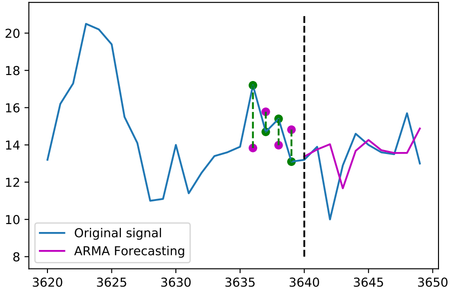
AR : Auto-Regressive modeling :

$$Y_t = \alpha + \alpha_1 Y_{t-1} + \alpha_2 Y_{t-2} + \ldots + \alpha_p Y_{t-p} + \varepsilon_1 \quad (1)$$

ARMA : Auto-Regressive Moving Average modeling :

$$Y_t = \alpha + \alpha_1 Y_{t-1} + \alpha_2 Y_{t-2} + \ldots + \alpha_p Y_{t-p} + \beta_1 \varepsilon_{t-1} + \beta_2 \varepsilon_{t-2} + \ldots + \beta_q \varepsilon_{t-q} \quad (2)$$

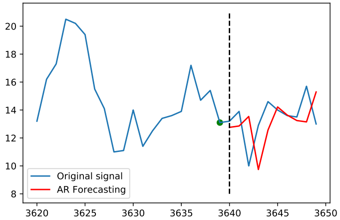


Complete Guide to Time Series Forecasting in Python, https://www.machinelearningplus.com/time-series/arima-model-time-series-forecasting-python/

ARMA (order 4,4) : 4 last measures are weighted by α & 4 errors ε are weighted by β to predict T

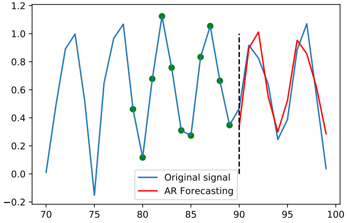
AR basic exemples & Periodicity discussion

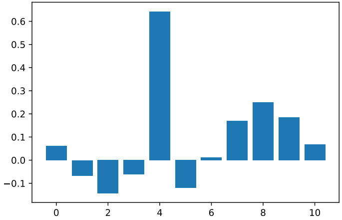
AR (order = 1) : a very intuitive model :



- Order 1 = delayed version of the original signal
- Periodic signals : high coefficients on the period

AR on periodic time series (order = 10) :





AR inference

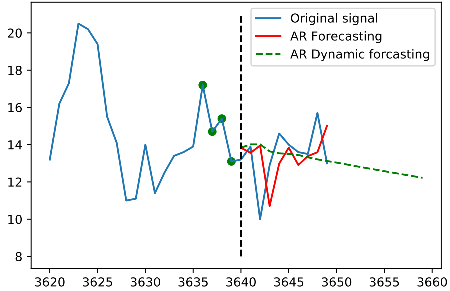
AR :

- Prediction at t :

$$\hat{y}_t = \alpha + \alpha_1 y_{t-1} + \alpha_2 y_{t-2} + \ldots + \alpha_p y_{t-p}$$

- Dynamic Prediction at t (from $t-2$) :

$$\hat{y}_t = \alpha + \alpha_1 \hat{y}_{t-1} + \alpha_2 y_{t-2} + \ldots + \alpha_p y_{t-p}$$



ARMA :

- Prediction at t :

$$y_t = \alpha + \alpha_1 y_{t-1} + \alpha_2 y_{t-2} + \ldots + \alpha_p y_{t-p} + \beta_1 \varepsilon_{t-1} + \beta_2 \varepsilon_{t-2} + \ldots + \beta_q \varepsilon_{t-q}$$

- Dynamic Prediction at t (from $t-2$) : ε_{t-1} can no longer be computed

ε_t that we can't compute are set to 0

Parameter optimization

Problem formulation (MSE) :

$$\mathcal{L} = \sum_t (y_t - \hat{y}_t)^2, \qquad \underset{\alpha,(\beta)}{\arg\min}\, \mathcal{L}$$

- AR problem admits a closed form solution (Yule Walker)
- ARMA is a convex problem that is solved by gradient descent

During training, $\hat{y}_t$ is estimated from real y_{t-p} values...
Our model is not dedicated to long term prediction.

Wikipedia,
https://en.wikipedia.org/wiki/Autoregressive_model

Finding AR optimal hyper-parameters

- Model selection : AR, ARMA, ARIMA
- Temporal window

Statistician

- Information Criterion : AIC (/ BIC)
- Akaike information criterion :

$$\text{AIC} = 2k - 2\ln(\mathcal{L})$$

k = nb estimated parameters

- Maximizing likelyhood
- while penalizing model complexity

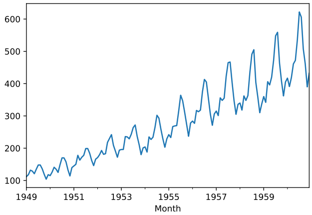
In practice : always very **low orders**

Computer scientist

- Cross validation (always)
  - Reconstruction criterion : MSE
- Estimating the generalization error on unseen data

ARIMA

- AR / ARMA approaches are dedicated to **stationary signals**
- Issue 1 : **measuring** stationarity
- Issue 2 : **improving** stationarity



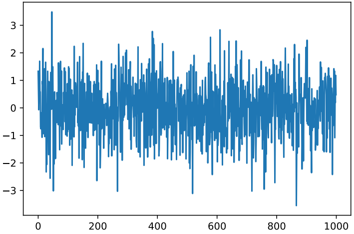
Hypothesis testing
(e.g. Dicky Fuller Test) :

```
Results of Dickey-Fuller Test:
Test Statistic                  0.815369
p-value                         0.991880
Critical Value (1%)            -3.482
Critical Value (5%)            -2.884
Critical Value (10%)           -2.579
```

⚠ Mind the definition of the null hypothesis
(Dickey-Fuller : null = non-stationary)

Stationarity & ARIMA model

- AR / ARMA approaches are dedicated to stationary signals
- Issue 1 : **measuring** stationarity
- Issue 2 : **improving** stationarity



Hypothesis testing (e.g. Dicky Fuller Test) :

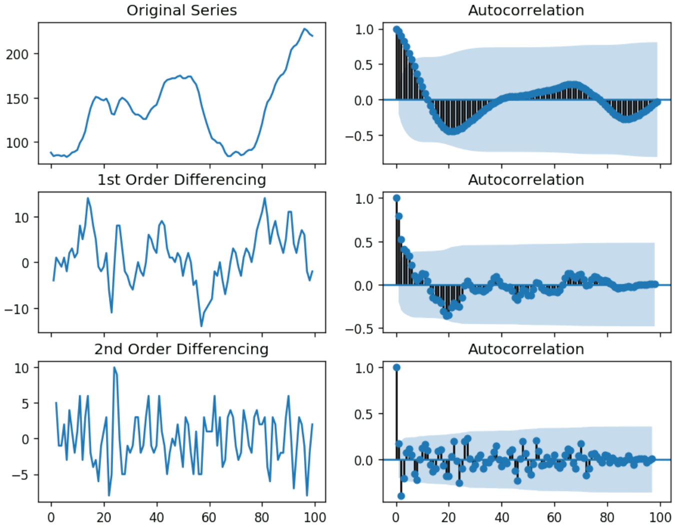
```
Results of Dickey-Fuller Test:
Test Statistic                -31.448939
p-value                         0.000000
Critical Value (1%)            -3.436
Critical Value (5%)            -2.864
Critical Value (10%)           -2.568
```

⚠ mind the definition of the null hypothesis (Dickey-Fuller : null = non-stationary)

Improving stationarity = signal differencing

Differencing the signal :

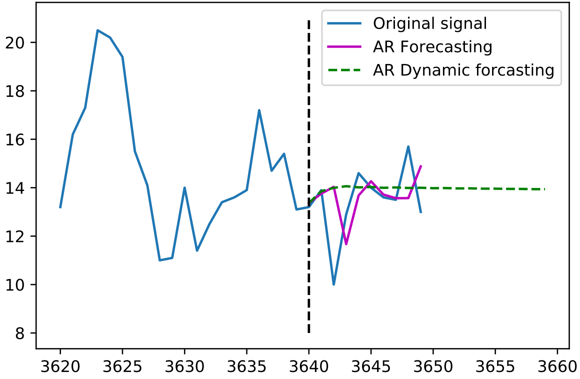
Order 1 :
$\delta_t = y_t - y_{t-1}$ instead of y_t
Order 2 :
$\delta_t^{(2)} = \delta_t - \delta_{t-1}$ instead of y_t



ARIMA :
Adding a (I)ntegrating parameter
= order of differencing

No autocorrelation = stationary signal

What can we expect from AR modeling in practice ?



In practice :

ARMA with low order = good local prediction

- Interesting modeling at $t+1$
- Flat prediction at $t+N$

Main issue :

no **seasonality** is taken into account ($\approx$ a way to model long term dependency)

Extracting trends & seasonality

1. Working at different scales : year, month, week, day, ... depending on the dataset
2. Seasonality extraction is done by convolution
   - denoting a trend t, a season s and a residue ε
     - period p must be provided
   - Additive model

$$y = t + s + \varepsilon$$

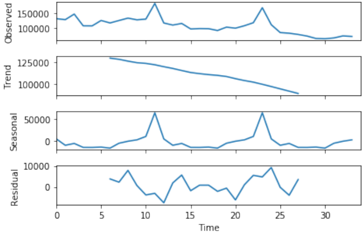
   - Multiplicative model

$$y = t \times s \times \varepsilon$$

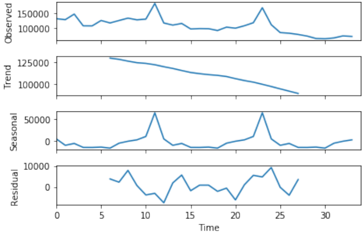
3. ARMA is performed on the residue

Time series Basics : Exploring traditional TS, G. Jagan
`https://www.kaggle.com/jagangupta/time-series-basics-exploring-traditional-ts`

Additive model :



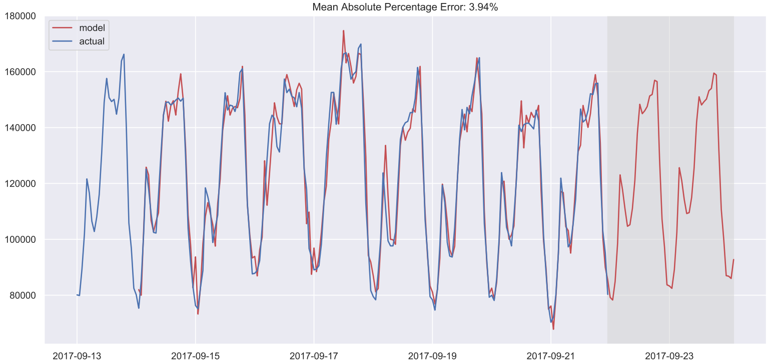
Multiplicative model :



SARIMA

Extension : Seasonality ARIMA

- Add a season length parameter
- Order(s) + Integration inside season
- + at the season level : $s_t = \alpha s_{t-1} + \ldots$



Adding seasonality enables long term better predictions.

ARMA tends to 0. Seasonality & trend remain reasonable.

AR/ARMA/SARIMA & exogenous factors

Give side informations about :

- the day, the hour,
- the weather condition...

AR :

$$\hat{y}_t = \alpha + \alpha_1 y_{t-1} + \alpha_2 y_{t-2} + \ldots + \alpha_p y_{t-p}$$

AR + exogenous factors $e_1, e_2, \ldots$:

$$\hat{y}_t = \alpha + \alpha_1 y_{t-1} + \alpha_2 y_{t-2} + \ldots + \alpha_p y_{t-p} + \beta_1 e_{t,1} + \beta_2 e_{t,2} + \ldots$$

$\Rightarrow$ you must provide exogenous factor for the inference on the test set

Exponential Filtering (Holt-Winters predictor)

A well known alternative to SARIMA :

- Order 1 :

$$\hat{y}_t = \alpha \cdot y_t + (1-\alpha) \cdot \hat{y}_{t-1}$$

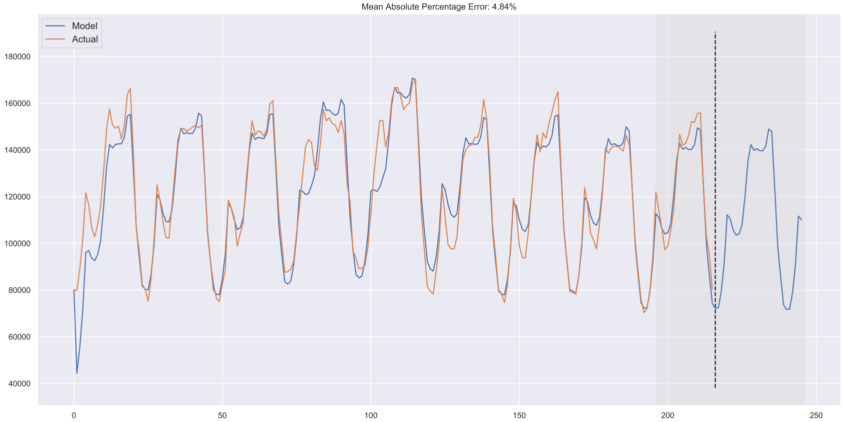
- Seasonality triple exponential filtering (=Holt-Winters)
  Prediction at horizon m, season $= s$, season length$=L$

$$\begin{aligned}
\text{1st order recursive model} : \ell_t &= \alpha\,(y_t - s_{t-L}) + (1-\alpha)\,(\ell_{t-1} + b_{t-1}) \\
\text{Differencing} : b_t &= \beta\,(\ell_t - \ell_{t-1}) + (1-\beta) b_{t-1} \\
\text{Seasonality} : s_t &= \gamma\,(y_t - \ell_t) + (1-\gamma) s_{t-L} \\
\text{Combination} : \hat{y}_{t+m} &= \ell_t + m b_t + s_{t-L+1+(m-1)\%L}
\end{aligned}$$

NB : the way to build this estimator is close to the gradient computation in ADAM

Exponential Filtering : results are close to SARIMA

Seasonality becomes more important than local modeling. . .



Greater horizon, simpler model

To look away an averaged season + trend is enough

Facebook Prophet model

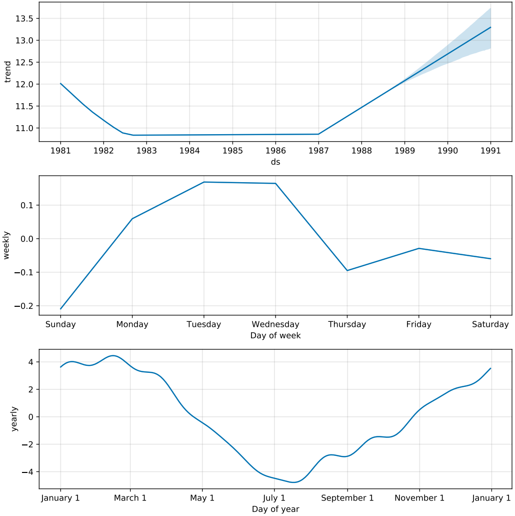
General formulation (Additive model) :

$$y(t) = g(t) + s(t) + h(t) + e(t)$$

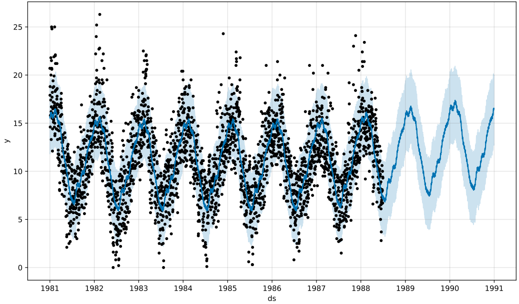
- $g(t)$: trends (for non periodic changes)
- $s(t)$: seasonality. In fact seasonality is multi-scale :
  - $s_h(t)$ hour, $s_d(t)$ day, $s_w(t)$ week, $s_m(t)$ month
- $h(t)$: holidays = prophet denomination for exogenous factors
- $e(t)$: residue

$\Rightarrow$ from statistics... Prophet $\approx$ SARIMA

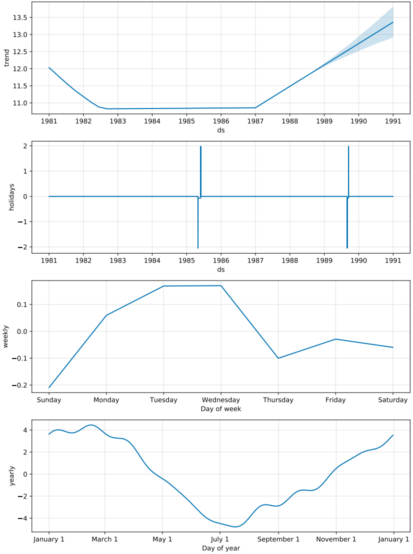
Prophet output



Australian daily minimum temperature



Prophet exogenous factor encoding



Simply define a `DataFrame` for your event & add it...

```
mod = Prophet(holidays=special_events)
#mod = Prophet()
```

Additional refinement :

- definition of overlapping special events
- possibilities to define additive or subtractive behaviour.

Prophet *vs* SARIMA

Prophet = a statistician tool in a computer science package

- more efficient (faster)
- more convenient ((almost) no parameter to set)
  - great integration with `pandas`
  - auto seasonality determination (relying on the calendar)
  - obvious counterpart : pandas is required
- better ML integration (scikit-learn / cross validation)

⇒ The statistical baseline to challenge ML approaches

Machine Learning Forecasting

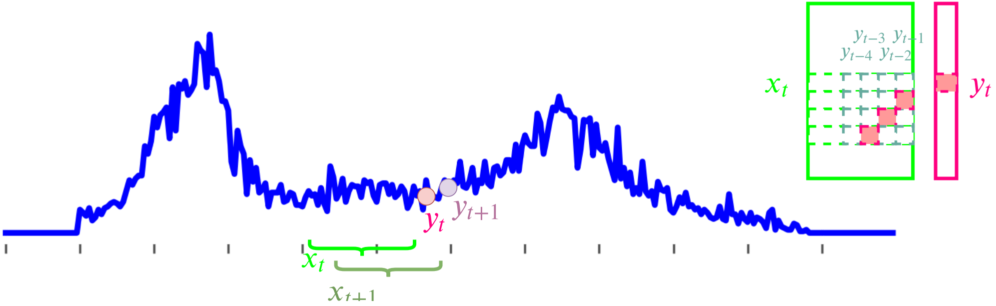
From AR to standard ML chains

- Linear (& non linear) regression : not only an interpolator but also a predictor
- feature engineering
  - Statistical features (tsfresh) + time freq
  - Sales prediction case
  - example of features
- SVM, XGboost, ... Or neural networks
- **Easy & cheap**

> some models will never be *production ready* as they demand too much time for the data preparation (for example, SARIMA),
> or require frequent re-training on new data (again, SARIMA),
> or are difficult to tune (good example - SARIMA),
> so it's very often much easier to select a couple of features from the existing time series and build a simple linear regression or, say, a random forest. Good and cheap.
>
> *Dmitry Sergeyev*

Rolling approaches

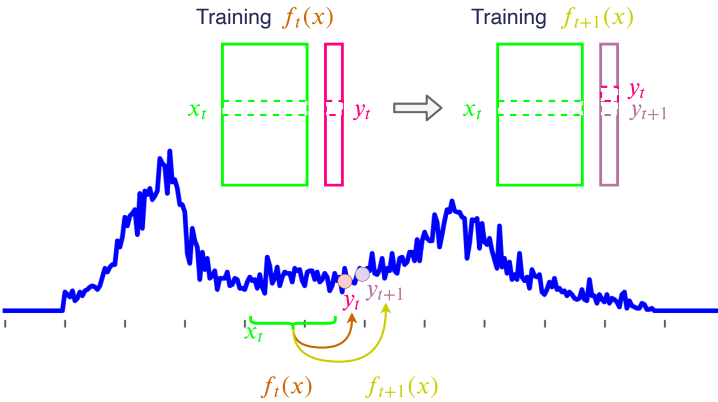
Introducing AR features in an ML environment :



Time	y	lag_6	lag_7	lag_8	lag_9	lag_10	lag_11	lag_12
2017-09-21 17:00:00	151790	132335.0	114380.0	105635.0	98860.0	97290.0	106495.0	113950.0
2017-09-21 18:00:00	155665	146630.0	132335.0	114380.0	105635.0	98860.0	97290.0	106495.0
2017-09-21 19:00:00	155890	141995.0	146630.0	132335.0	114380.0	105635.0	98860.0	97290.0

Predict further in time

- how to do it with ARMA ?
  - Train your model at $t+1$ (always)
  - Apply learnt coefficient α on prediction $\hat{y}$
  - Expect poor results (without seasonality)
- how to do it with ML chain
  - Learning to predict further directly
  - Intrinsically compatible with exogenous variables



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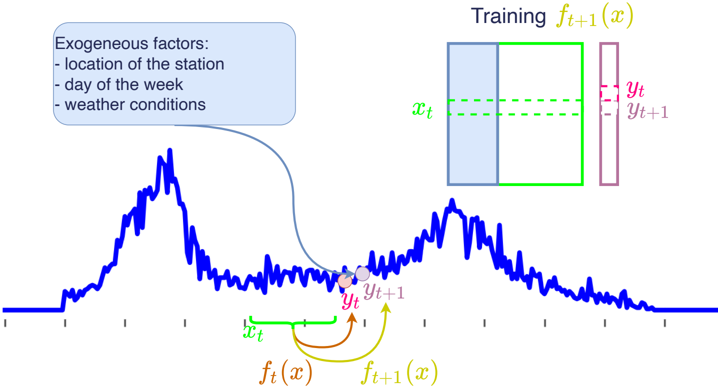
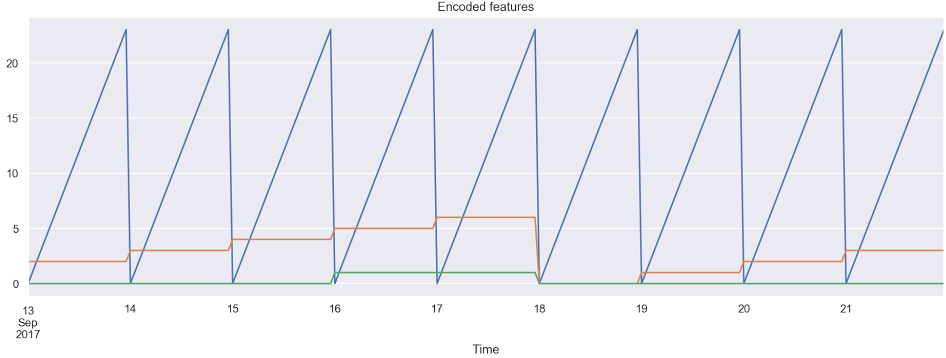


Exogenous factors / Feature engineering

Exogenous factors is straightforward in ML : just add features in the dataset

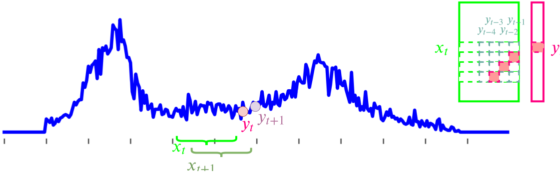
- Another way to encode seasonality
- Using pandas to catch up prophet functions
  - Types of days
  - Hours...

Example of time encoding : hour, day, week-end :



Feature engineering

- Depending on the application ⇒ discussions with experts
  [Often] more expert features ⇒ more performance
- Local statistics computations
  - Statistic moment
  - Frequency / power spectral density...
  - `tsfresh`
    - Hundreds of features...
    - ... & test of relevant ones
- Classical feature engineering
  - Feature clustering, ...
- Target encoding
  - e.g. Average value on Monday / weekday / ...



⇒ `pandas` is required for rolling, date reading & target encoding...
`pandas` is essential for timeseries !

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  [Often] more expert features ⇒ more performance
- Local statistics computations
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  - Frequency / power spectral density...
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- Target encoding
  - e.g. Average value on Monday / weekday / ...

`abs_energy` (x)	Returns the absolute energy of the time se
`absolute_sum_of_changes` (x)	Returns the sum over the absolute value of
`agg_autocorrelation` (x, param)	Calculates the value of an aggregation func
`agg_linear_trend` (x, param)	Calculates a linear least-squares regression
`approximate_entropy` (x, m, r)	Implements a vectorized Approximate entr
`ar_coefficient` (x, param)	This feature calculator fits the unconditiona
`augmented_dickey_fuller` (x, param)	The Augmented Dickey-Fuller test is a hyp
`autocorrelation` (x, lag)	Calculates the autocorrelation of the specif
`binned_entropy` (x, max_bins)	First bins the values of x into max_bins equ
`c3` (x, lag)	This function calculates the value of
`change_quantiles` (x, ql, qh, isabs, f_agg)	First fixes a corridor given by the quantiles
`cid_ce` (x, normalize)	This function calculator is an estimate for a

⇒ `pandas` is required for rolling, date reading & target encoding...
`pandas` is essential for timeseries !

Sales prediction use case

- Nature of the data
  - Shops
  - Items
- Target :
  - Fine grain : predicting the amount of each items in each Shops
  - General : sales revenue

Idea : extracting features for all objects

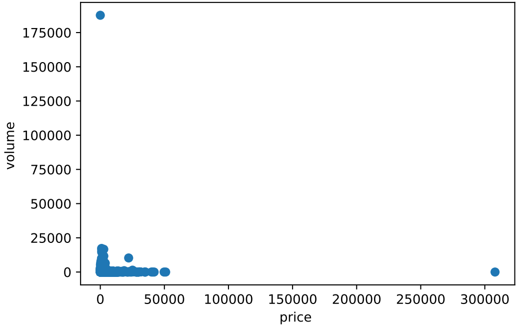
$\Rightarrow$ Exploit ML plasticity $\Leftrightarrow$ hard to model with AR

K. Yacovlev, Kaggle notebook, 2019
https://www.kaggle.com/kyakovlev/1st-place-solution-part-1-hands-on-data

Sales prediction use case : classical features

- Items (aggregated over all shops)
  - Item category (from expert, from name, ...)
  - Item general trends
  - Binary : Is deprecated / Is new
  - Price/volume categorization :
    - removing (or separating outliers)
    - linspace separation
    - histogram
    - clustering
- Shops
  - Same features + co-clustering with items
- Time
  - Black Friday, holidays, ...

Items prices & volumes



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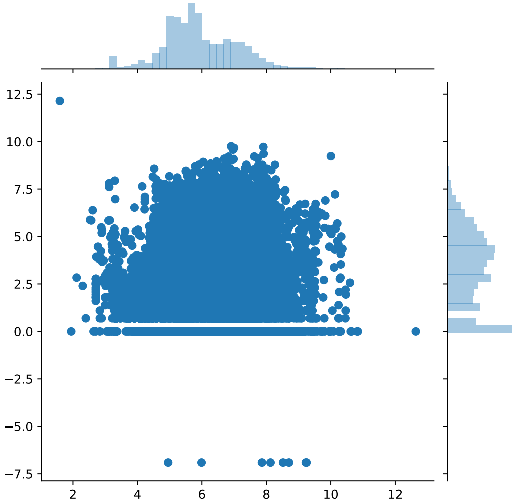
Items **log** prices & volumes



Sales prediction use case : mono/multivariate approach

- Single shop prediction
  - with some features computed on multiple shops
- Multiple shop prediction
- Predicting all item per shop sales

- Feature engineering makes monovariate prediction very strong
- Deep learning (try to) tackles multivariate prediction
  - To extract relevant feature automatically
  - To find fine correlation between shop/item dynamics

Variable weights normalization & interpretations

- Do not forget to normalize your data
  - Always in ML... But really mandatory when dealing with heterogenous variables
- Model introspection is always a good Idea

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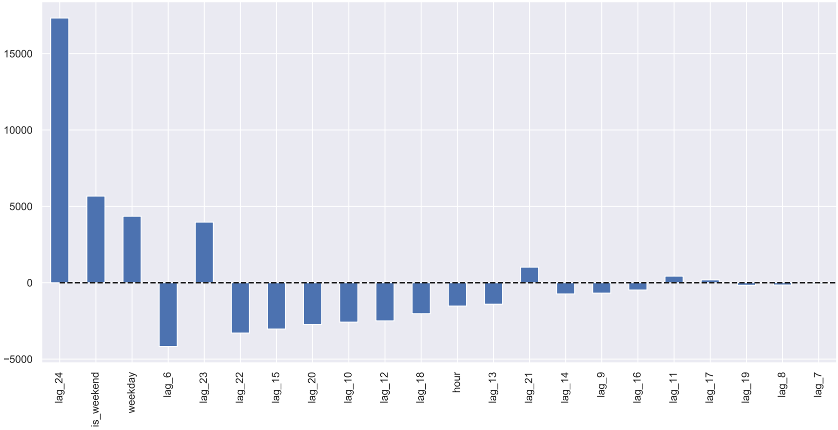
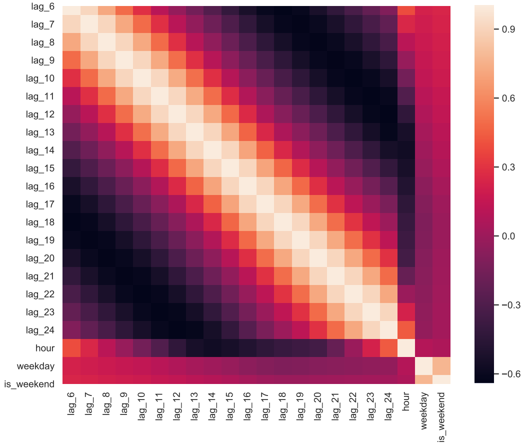


Regularization & variable selection

Extracting many features (or even several) lead to this kind of data shape :



- Ridge/regularized logistic regression
  - at least, to reduce the bad impact of correlated variables
- LASSO/Variable selection procedure
  - Reducing the number of features
  - scikit-learn...

XGBoost (everything ?)

A nice algorithm…

And a **wonderful** implementation !

- like libSVM, word2vec, …

Unsurprisingly $\Rightarrow$ Yes, it is a good idea

- Unmatched performance/development-time ratio
  - Surprising resistance to overfitting
  - Efficiency of the default setting
- Model introspection :
  let's exploit all available functions

Amjad Abu-Rmileh, The Multiple faces of *Feature importance* in XGBoost
`https://towardsdatascience.com/be-careful-when-interpreting-your-features-impor`

Metrics & Anomalies

Metrics – How to evaluate if our predictions are relevant ?

R squared

s_y^2 = Empirical variance of Y :

$$s_y^2 = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - \overline{y})^2 + \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

s_y^2 = explained variance + residual variance

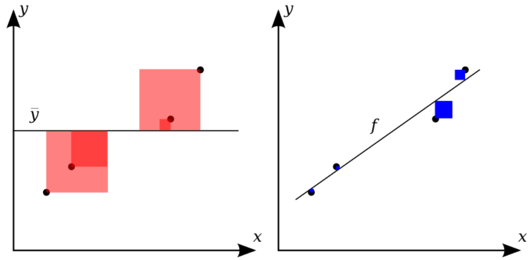
$$R^2 = \frac{\sum_i(\hat{y}_i - \overline{y})^2}{\sum_i(y_i - \hat{y}_i)^2} = \frac{\text{explained variance}}{\text{residual variance}}$$

Metrics – How to evaluate if our predictions are relevant ?

R squared

coefficient of determination (in econometrics it can be interpreted as a percentage of variance explained by the model)

$$R^2 = 1 - \frac{SS_{residue}}{SS_{total}}$$



1 : all variance of the data explained $\Rightarrow$ best results

0 : worst model

Classical metrics

- Mean Absolute error

$$MAE = \frac{\sum_{i=1}^{n} |y_i - \hat{y}_i|}{n}$$

- Median Absolute Error (robust to outliers)

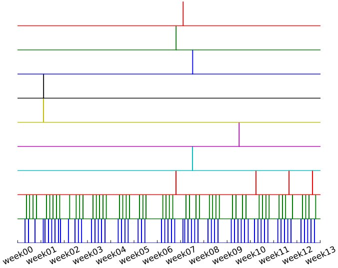
$$MedAE = \text{median}(|y_1 - \hat{y}_1|, \ldots, |y_n - \hat{y}_n|)$$

- Mean Absolute Percentage Error

$$MAPE = \frac{100}{n} \sum_{i=1}^{n} \frac{|y_i - \hat{y}_i|}{y_i}$$

Choose the metric adapted to your data to evaluate...
Even if you (often) use MSE as a learning criterion

Side effects with MAPE, definition of SMAPE



Working on sparse data (e.g. validations of a single user in public transportation)
Lots of 0 in the ground truth :

- $MAPE = \frac{100}{n}\sum_{i=1}^{n}\frac{|y_i - \hat{y}_i|}{y_i}$ diverges

Solutions :

- Rough aggregation over time to reduce sparseness
- Dedicated metrics
- ... SMAPE :

$$\mathrm{SMAPE}_1 = \frac{100\%}{n}\sum_{t=1}^{n}\frac{|y_t - \hat{y}_t|}{(|\hat{y}_t| + |y_t|)/2} \quad \text{or} \quad \mathrm{SMAPE}_2 = \frac{\sum_{t=1}^{n}|y_t - \hat{y}_t|}{\sum_{t=1}^{n}(\hat{y}_t + y_t)}$$

Not magic... but sometimes robust enough to build an operational system

Anomaly definition

Something that is not supposed to append. Different cases :

- Outlier / error of measurement
- Distance between observations and predictions
- Anomaly tag labeled in the dataset

$\Rightarrow$ we focus on distances

Required for in-depth evaluation & for model monitoring in production

Anomaly detection : proposed implementation

- Computing bounds very easily :

```
mae = mean_absolute_error(series[window:], prediction[window:])
deviation = np.std(series[window:] - prediction[window:])
lower_bond = prediction - (mae + scale * deviation)
upper_bond = prediction + (mae + scale * deviation)
```

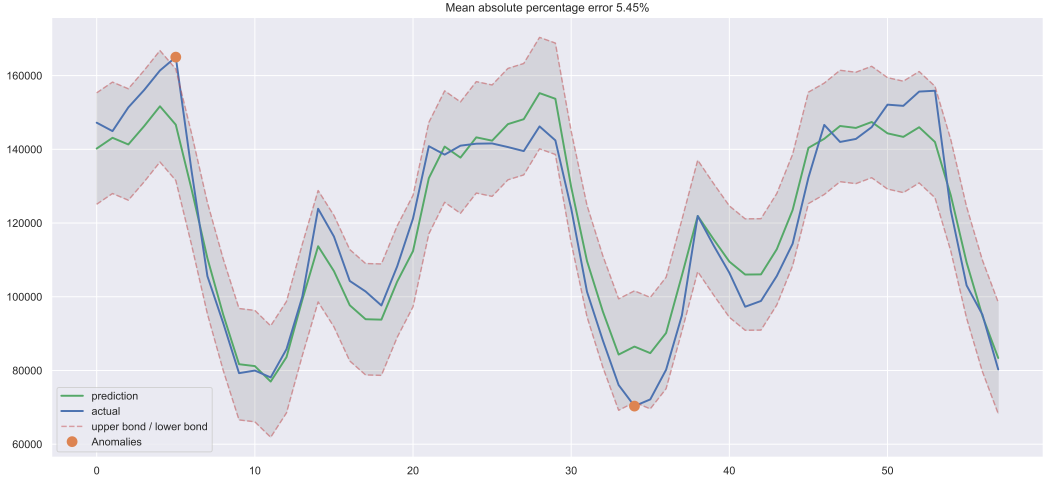
`scale = 1.96` (often)

- A more robust approach (still easy to implements)

```
cv = cross_val_score(model, series[window:], target[window:],
                     scoring="neg_mean_absolute_error")
mae = cv.mean() * (-1)
deviation = cv.std()
lower_bond = prediction - (mae + scale * deviation)
upper_bond = prediction + (mae + scale * deviation)
```

`scale = 1.96` (often)

Expected results

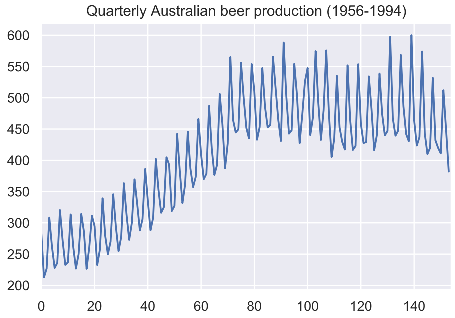


Anomalies are prediction outside the confidence bounds

Pitfalls in ML for time series

Case 1 : trend change

Difficult case : what happen when the test distribution diverges from the training one ?



Predicting on long term basis with SARIMA :
trend + season

Autralian beer production : typical series with abrupt change

Time Series Nested Cross-Validation, Courtney Cochrane
https://towardsdatascience.com/time-series-nested-cross-validation-76adba623eb9

Case 1 : trend change

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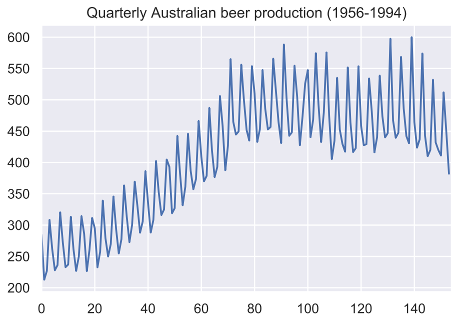

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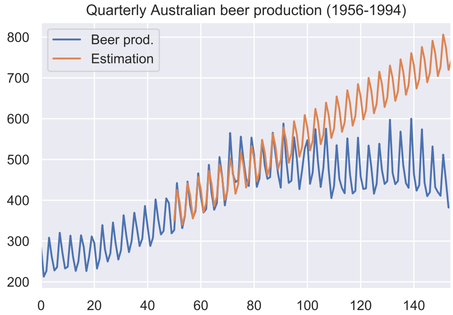

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Case 1 : Detection & Resolution

+ A good example : trend may change abruptly in many situations
– Who has ever use the same (SARIMA) model 10 years long without :
    - retraining
    - feeding the model with real data regularly
- A particular instance of iid hypothesis failure : very classical in ML

Detection

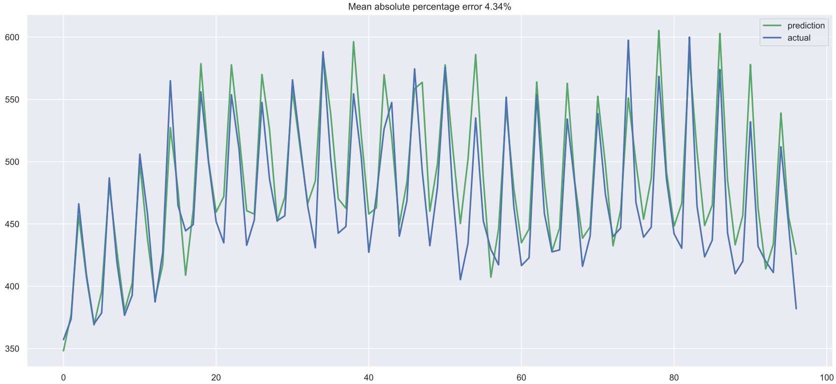
- Human monitoring
- Anomaly detection
- Change detection

Resolution

- Re-train models regularly
- Evaluate your model on recent Data (even in production)
    - Perform anomaly detection, raise alarms

Case 1 : getting closer to real case

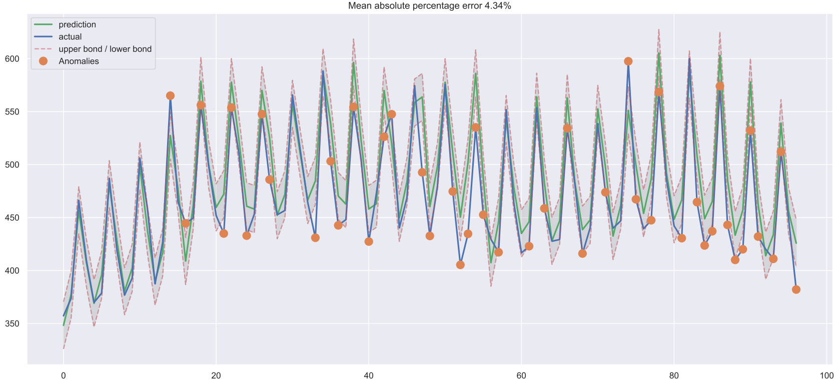
- Keep the same model on a long term basis...
- ... But feed it with new data at each time step



Difficult to estimate the quality of the prediction

Case 1 : getting closer to real case

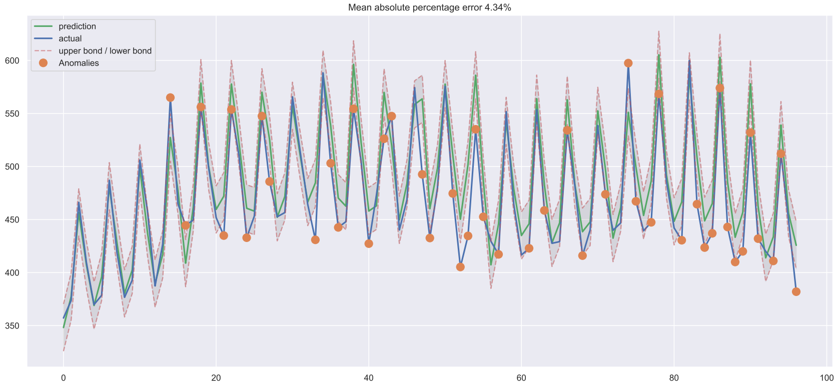
- Keep the same model on a long term basis...
- ... But feed it with new data at each time step



⇒ Adding confidence bounds & alarm detection

Case 1 : getting closer to real case

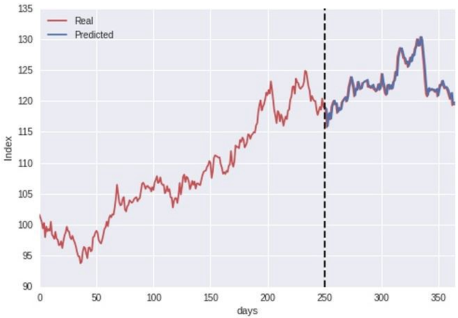
- Keep the same model on a long term basis...
- ... But feed it with new data at each time step

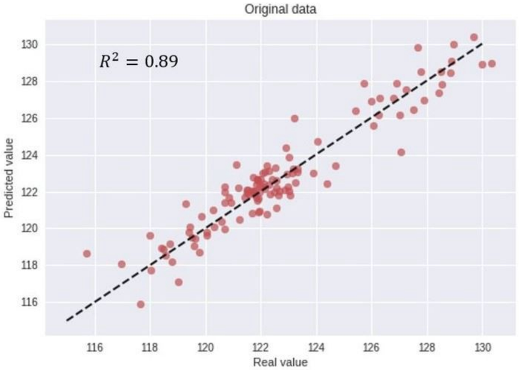


Alterative : Monitoring the results of a strong baseline

$\Rightarrow$ Results will converge between advanced model & baseline

Case 2 : a pretty good forecast





When you look at it from afar

How (not) to use Machine Learning for time series forecasting : Avoiding the pitfalls, Vegard Flovik
https://towardsdatascience.com/how-not-to-use-machine-learning-for-time-series-forecasting-avo

Case 2 : a pretty good forecast

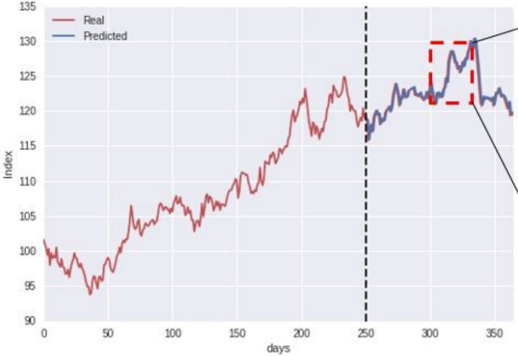
But actually :

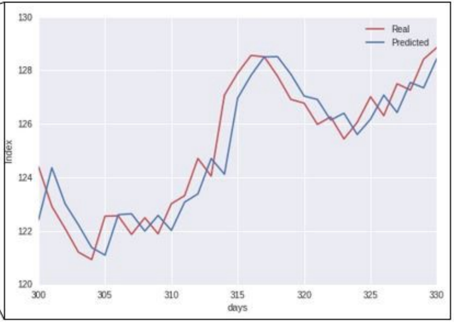
- Data are generated from a random walk...

⇒ it can't be predicted !

How (not) to use Machine Learning for time series forecasting : Avoiding the pitfalls, Vegard Flovik
https://towardsdatascience.com/how-not-to-use-machine-learning-for-time-series-forecasting-avo

Case 2 : look at the details

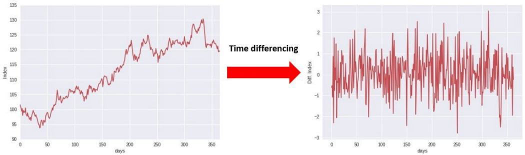


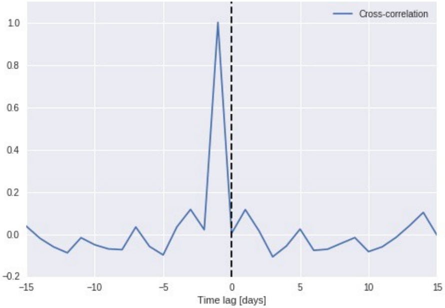


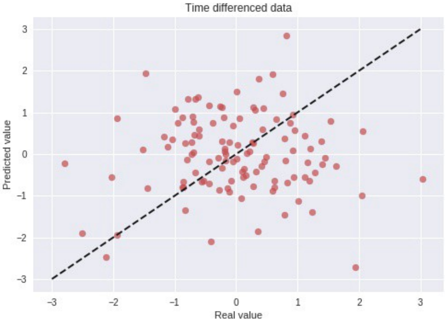
A very basic solution : $\hat{y}_t = y_{t-1}$

Case 2 : what was wrong ? How to detect this case ? [Statistics]

- Do not use ARMA on non stationary signals
- Measure cross-correlation between y and $\hat{y}$.

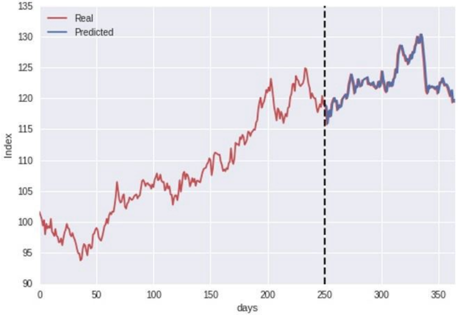






Case 2 : what was wrong ? How to detect this case ? [Computer science]

Always compare a predictor to a strong baseline



- Choose the good baselines
  - Linear ? $\Rightarrow$ not sufficient
  - Time series $\Rightarrow$ at least
    - Previous value : $\hat{y}_t = y_{t-1}$
    - Moving average : $\hat{y}_t = \frac{1}{T} \sum_i y_{t-i}$

1. Compare the results in CV...
2. And the standard deviation on the results.

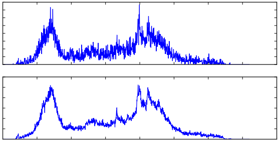
Baselines : a more comprehensive list

General baseline for time series :

- Previous value : $\hat{y}_t = y_{t-1}$
- Moving average : $\hat{y}_t = \frac{1}{T}\sum_i y_{t-i}$
- Predict always the most frequent value (rarely efficient on time series)

Seasonal data :

- Take one averaged season
  - e.g. in public transportation : average weekday or average Monday $=$ prediction for every Monday
  - Strong baseline on specific dataset
  - **Very** strong baseline beyond $T+1$



One Wednesday / averaged Wednesday on a particular subway station

ML classical baseline

- Linear model
- K-nn : all $y_{t-1} = \alpha$ lead to $y_t = \beta$

Case 3 : In-sample evaluation

Classical block cross-validation = seeing the future

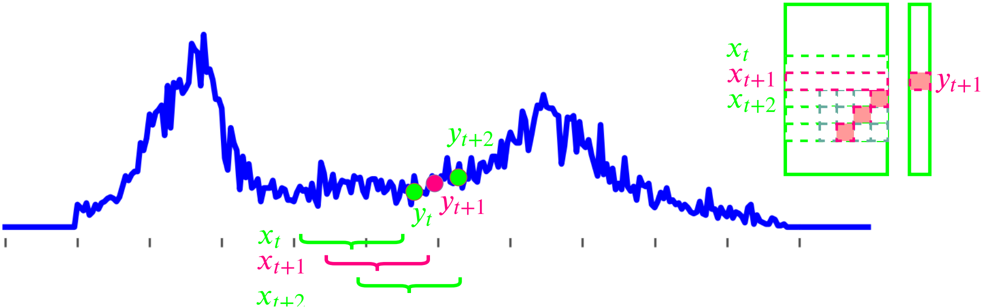
- cheating on any unpredictable (/ not modeled) trends
  - Difficult prediction problem turns into to a simpler interpolation problem
- side effect at the beginning/end of each test split (cf next slide)

Iteration 1	Test	Train	Train	Train	Train
Iteration 2	Train	Test	Train	Train	Train
Iteration 3	Train	Train	Test	Train	Train
Iteration 4	Train	Train	Train	Test	Train
Iteration 5	Train	Train	Train	Train	Test

Leonard J. Tashman, Int. Jour. of Forecasting, 2000
Out-of-sample tests of forecasting accuracy : an analysis and review

Case 3 : In-sample evaluation & information leak

Shuffled cross validation : test samples are surrounded by training ones

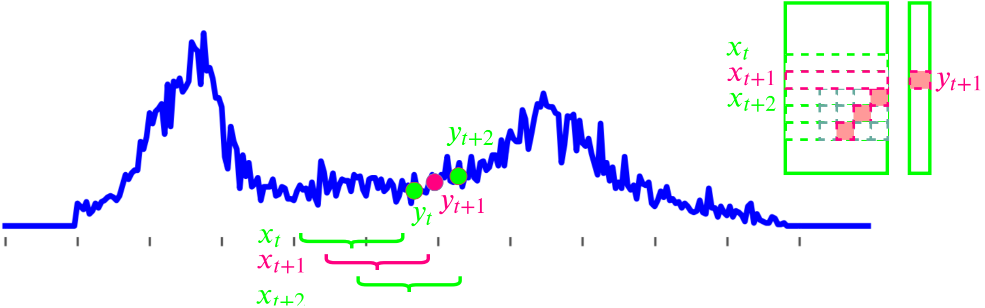


- Target x_{t+1} : find the most correlated points $\{x_c\}$ in the training set
- Add criterion to detect the better one regarding temporal evolution
- Predict $x_c^{\star}[end]$

$\Rightarrow$ it can even work to predict at $T + N$!

Case 3 : In-sample evaluation & information leak

Shuffled cross validation : test samples are surrounded by training ones



The only thing evaluated in this procedure is :

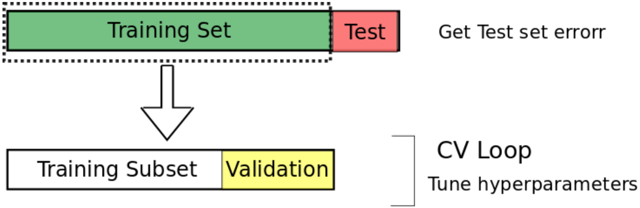
Is y_{t+1} close to y_t most of the time ?

... And it is often the case !

$\Rightarrow$ You may obtain a prediction accuracy better that the intrinsic noise level !

Case 3 : In-sample / Out-of-sample evaluation [single series]

Switching to out-of-sample evaluation :



Note : to optimize your parameters, you have to use a validation set at the end of the training set.

Leonard J. Tashman, Int. Jour. of Forecasting, 2000
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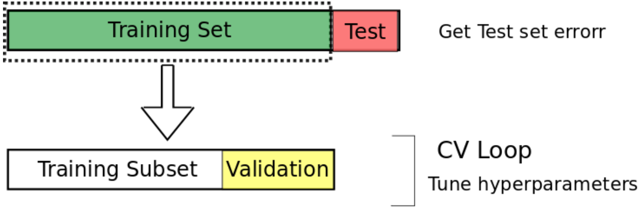

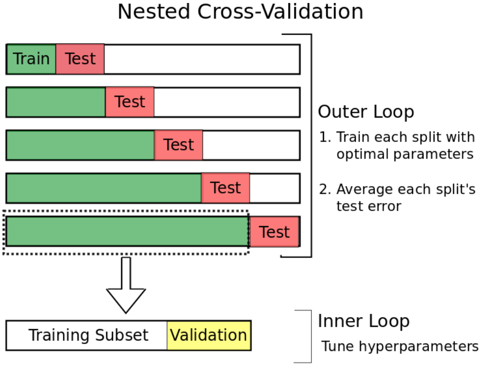

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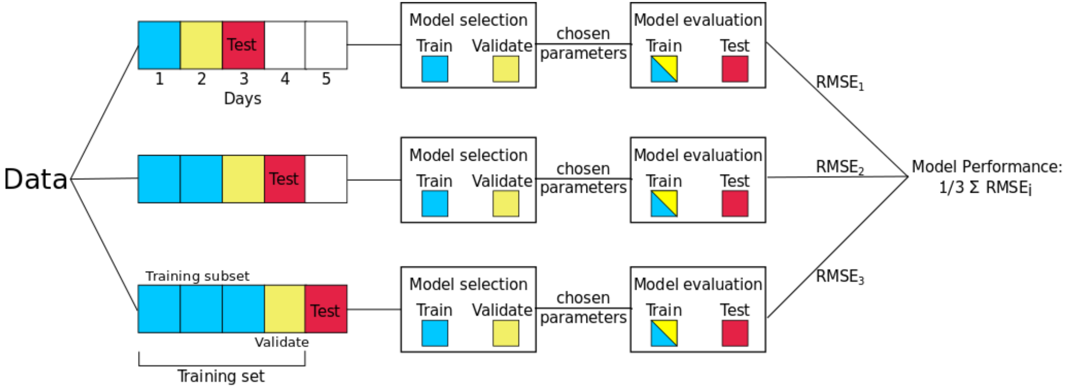
Leonard J. Tashman, Int. Jour. of Forecasting, 2000
Out-of-sample tests of forecasting accuracy : an analysis and review

Case 3 : Complete Nested Cross-Validation procedure [single series]



Good news : it is already implemented in scikit-learn. ⇒ just use it !

```
from sklearn.model_selection import TimeSeriesSplit
```

Case 3 : Nested Cross Validation over a population

Interdependent samples

e.g. evolution of the temperature in multiple cities / sales in different shops

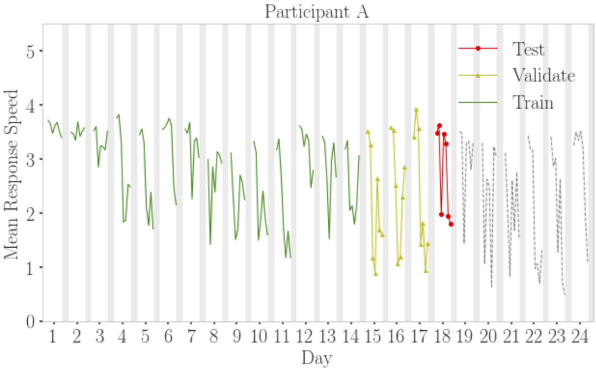
- Apply the Nested CV on all samples
- Make sure that Train/test frontier corresponds to an absolute time-stamp

Independent samples

e.g. Patient response to a treatment

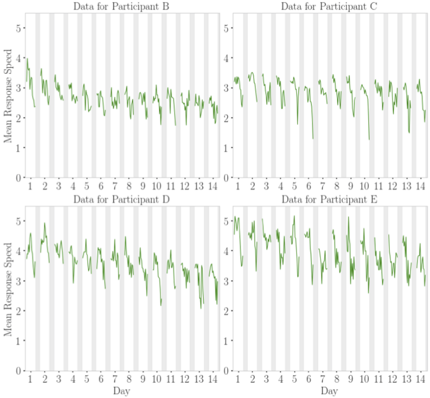
Case 3 : Nested Cross Validation over a population

Interdependent samples



Independent samples

e.g. Patient response to a treatment



Case 3 : Detect temporal information leak

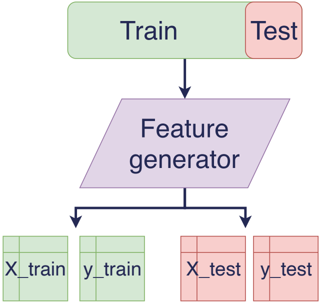
Nested cross validation **is supposed to** enable you to detect information leak...

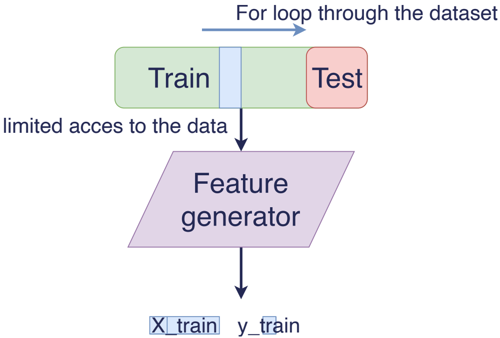
One case remains critical

Creating a **leaking feature** may be difficult to detect.

e.g.

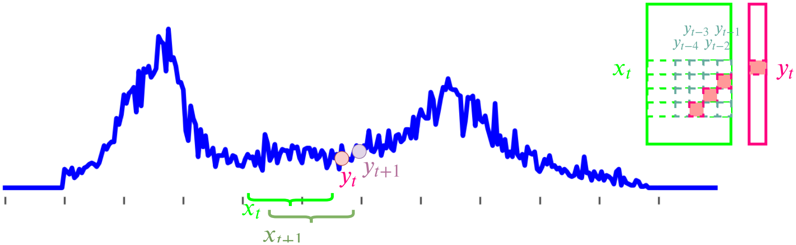
- An aggregation of values overflowing in the future of the sample
  - Target encoding
- Uncontrolled feature (from tsfresh)





⇒ Even if we don't like for loop, even if it is less convenient...

Case 4 : Normalization of the lag variables (not the contextual ones)



As in any machine learning use case, dealing with time series requires normalization :

- Normalization by columns
  - ⇒ Great impact of future measurements on the data
  - ⇒ Destruction of the temporal dependencies
- Normalization by line
  - Impact of the future measurements on the data
  - ... But limited impact
    - Normalizing by the max
    - Even better : normalizing by the 99% percentile
    - Very stable information that could have been given by an expert

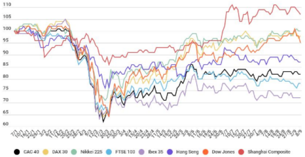
Conclusion

Important factors in time series prediction

- Analysing local dynamics = Auto Regressive models
  - $\Rightarrow$ Useful for close prediction
  - $\Rightarrow$ Not sufficient for mid/long term prediction
- Distinguish : past values ; trends & seasonality ; exogenous factors...
  - $\Rightarrow$ Impact of specific pattern ?
  - $\Rightarrow$ Bridge between time series prediction $\Leftrightarrow$ source separation
- Pitfalls are numerous...
  - $\Rightarrow$ Don't forget your statistical references
  - $\Rightarrow$ Always consider a XGBoost/Random Forest option... and compare it to the right baselines
  - $\Rightarrow$ Beware of magical features / unrealistic good prediction (!)

Global picture

python



Modèles AR — PROPHET, statsmodels, NumPy, pandas, matplotlib

Modèles ML : SVM, XGB — scikit learn, XGBoost

Modèles DL : CNN, RNN — PyTorch, NVIDIA CUDA

Incremental

- Different approaches, different paradigms/syntaxes
- Different costs, different expectations
- Different hardware supports
- Great tools... But remind the time frame