1st place solution

posted in Web Traffic Time Series Forecasting 3 months ago

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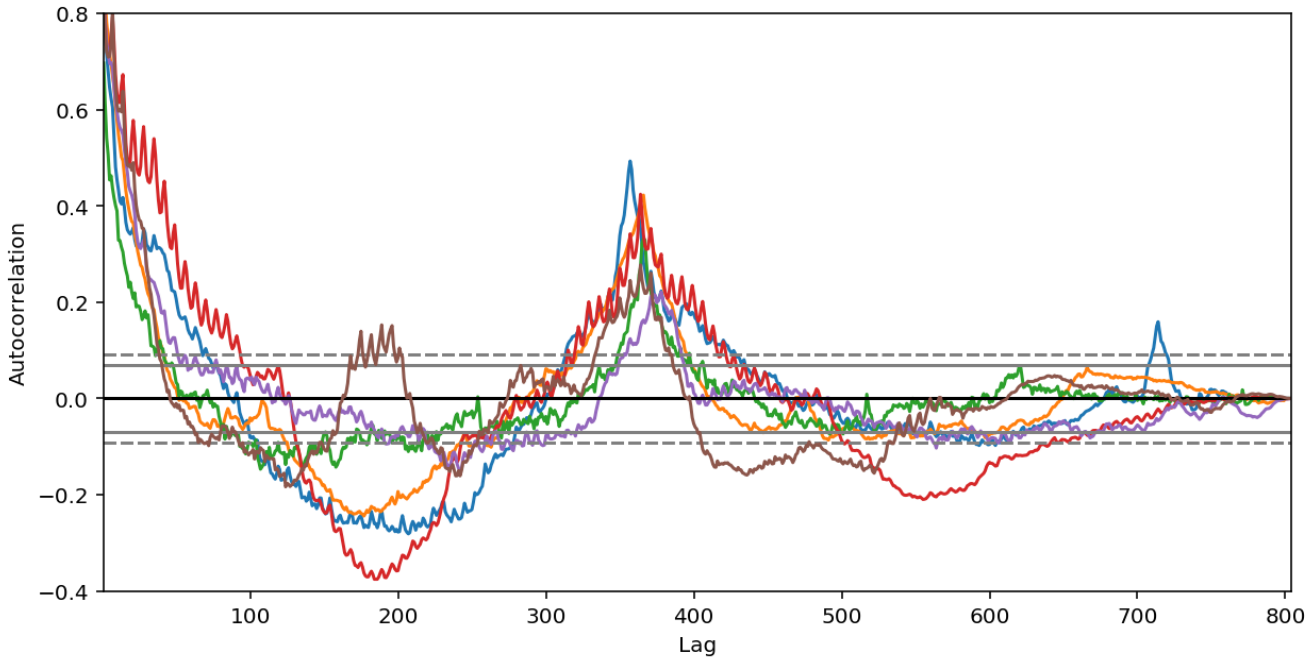
TL;DR this is seq2seq model with some additions to utilize year-to-year and quarter-to-quarter seasonality in data.

Model code: https://github.com/Arturus/kaggle-web-traffic

There are two main information sources for prediction:

1. Local features. If we see a trend, we expect that it will continue (AutoRegressive model), if we see a traffic spike, it will gradually decay (Moving Average model), if wee see more traffic on holidays, we expect to have more traffic on holidays in the future (seasonal model).
2. Global features. If we look to autocorrelation plot, we'll notice strong year-to-year autocorrelation and some quarter-to-quarter autocorrelation.

The good model should use both global and local features, combining them in a intelligent way.



I decided to use RNN seq2seq model for prediction, because:

1. RNN can be thought as a natural extension of well-studied ARIMA models, but much more flexible and expressive.
2. RNN is non-parametric, that's greatly simplifies learning. Imagine working with different ARIMA parameters for 145K timeseries.

3. Any exogenous feature (numerical or categorical, time-dependent or series-dependent) can be easily injected into the model
4. seq2seq seems natural for this task: we predict next values, conditioning on joint probability of previous values, including our past predictions. Use of past predictions stabilizes the model, it learns to be conservative, because error accumulates on each step, and extreme prediction at one step can ruin prediction quality for all subsequent steps.
5. Deep Learning is all the hype nowadays

Feature engineering

I tried to be minimalistic, because RNN is powerful enough to discover and learn features on its own.

Model feature list:

- *pageviews* (spelled as 'hits' in the model code, because of my web-analytics background). Raw values transformed by log1p() to get more-or-less normal intra-series values distribution, instead of skewed one.
- *agent*, *country*, *site* - these features are extracted from page urls and one-hot encoded
- *day of week* - to capture weekly seasonality
- *year-to-year autocorrelation*, *quarter-to-quarter autocorrelation* - to capture yearly and quarterly seasonality strength.
- *page popularity* - High traffic and low traffic pages have different traffic change patterns, this feature (median of pageviews) helps to capture traffic scale. This scale information is lost in a *pageviews* feature, because each pageviews series independently normalized to zero mean and unit variance.
- *lagged pageviews* - I'll describe this feature later

Feature preprocessing

All features (including one-hot encoded) are normalized to zero mean and unit variance. Each *pageviews* series normalized independently.

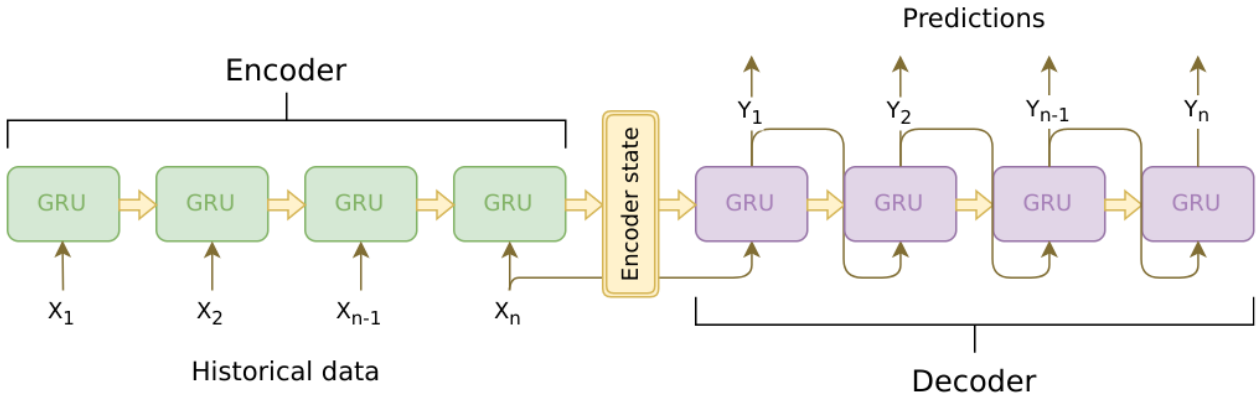
Time-independent features (autocorrelations, country, etc) are "stretched" to timeseries length i.e. repeated for each day by `tf.tile()` command.

Model trains on random fixed-length samples from original timeseries. For example, if original timeseries length is 600 days, and we use 200-day samples for training, we'll have a choice of 400 days to start the sample.

This sampling works as effective data augmentation mechanism: training code randomly chooses starting point for each timeseries on each step, generating endless stream of almost non-repeating data.

Model core

Model has two main parts: encoder and decoder.



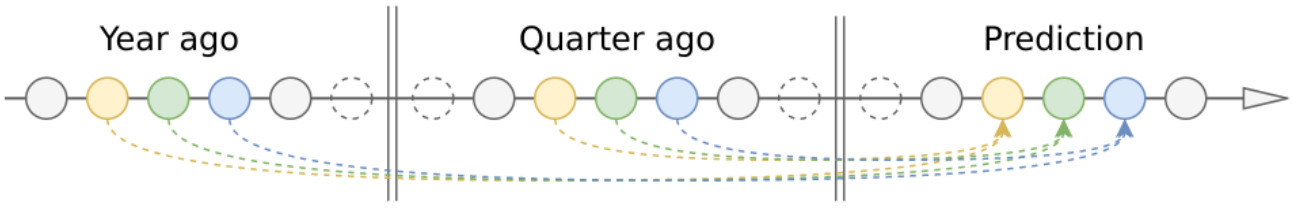
Encoder is cuDNN GRU. cuDNN works much faster (5x-10x) than native Tensorflow RNNCells, at the cost of some inconvenience to use and poor documentation.

Decoder is TF `GRUBlockCell` , wrapped in `tf.while_loop()` construct. Code inside the loop gets prediction from previous step and appends it to the input features for current step.

Working with long timeseries

LSTM/GRU is a great solution for relatively short sequences, up to 100-300 items. On longer sequences LSTM/GRU still works, but can gradually forget information from the oldest items. Competition timeseries is up to 700 days long, so I have to find some method to "strengthen" GRU memory.

My first method was to use some kind of *attention*. Attention can bring useful information from a distant past to the current RNN cell. The simplest yet effective attention method for our problem is a fixed-weight sliding-window attention. There are two most important points in a distant past (taking into account long-term seasonality): 1) year ago, 2) quarter ago.



I can just take encoder outputs from `current_day - 365` and `current_day - 90` timepoints, pass them through FC layer to reduce dimensionality and append result to input features for decoder. This solution, despite of being simple, considerably lowered prediction error.

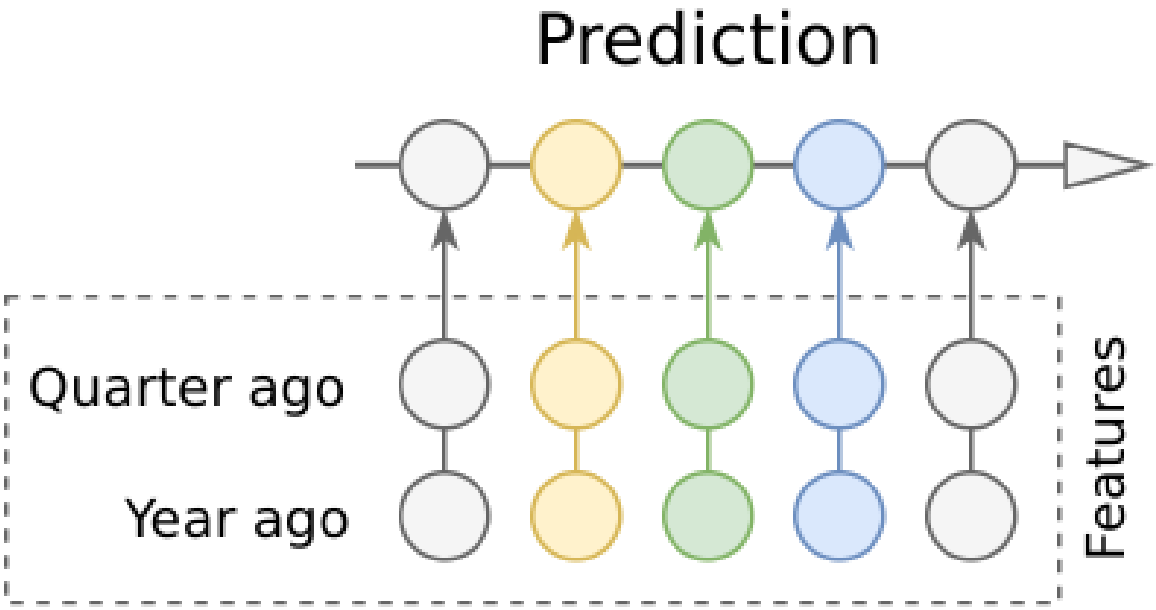
Then I averaged important points with their neighbors to reduce noise and compensate uneven intervals (leap years, different month lengths): `attn_365 = 0.25 * day_364 + 0.5 * day_365 + 0.25 * day_366`

Then I realized that `0.25,0.5,0.25` is a 1D convolutional kernel (length=3) and I can automatically learn bigger kernel to detect important points in a past.

I ended up with a monstrous attention mechanism, it looks into 'fingerprint' of each timeseries (fingerprint produced by small ConvNet), decides which points to attend and produces weights for big convolution kernel. This big kernel, applied to decoder outputs, produces attention features for each prediction day. This monster is still alive and can be found in a model code.

Note, I did'nt used classical attention scheme (Bahdanau or Luong attention), because classical attention should be recalculated from scratch on every prediction step, using all historical datapoints. This will take too much time for our long (~2 years) timeseries. My scheme, one convolution per all datapoints, uses same attention weights for all prediction steps (that's drawback), but much faster to compute.

Unsatisfied by complexity of attention mechanics, I tried to remove attention completely and just take important (year, halfyear, quarter ago) datapoints from the past and use them as an additional features for encoder and decoder. That worked surprisingly well, even slightly surpassing attention in prediction quality. My best public score was achieved using only lagged datapoints, without attention.



Additional important benefit of lagged datapoints: model can use much shorter encoder without fear of losing information from the past, because this information now explicitly contained in features. Even 60-90 days long encoder still gives acceptable results, in contrast to 300-400 days required for previous models. Shorter encoder = faster training and less loss of information

Losses and regularization

SMAPE (target loss for competition) can't be used directly, because of unstable behavior near zero values (loss is a step function if truth value is zero, and not defined, if predicted value is also zero).

I used smoothed differentiable SMAPE variant, which is well-behaved at all real numbers:

```
epsilon = 0.1
summ = tf.maximum(tf.abs(true) + tf.abs(predicted) + epsilon, 0.5 + epsilon)
smape = tf.abs(predicted - true) / summ * 2.0
```

Another possible choice is MAE loss on `log1p(data)`, it's smooth almost everywhere and close enough to SMAPE for training purposes.

Final predictions were rounded to the closest integer, negative predictions clipped at zero.

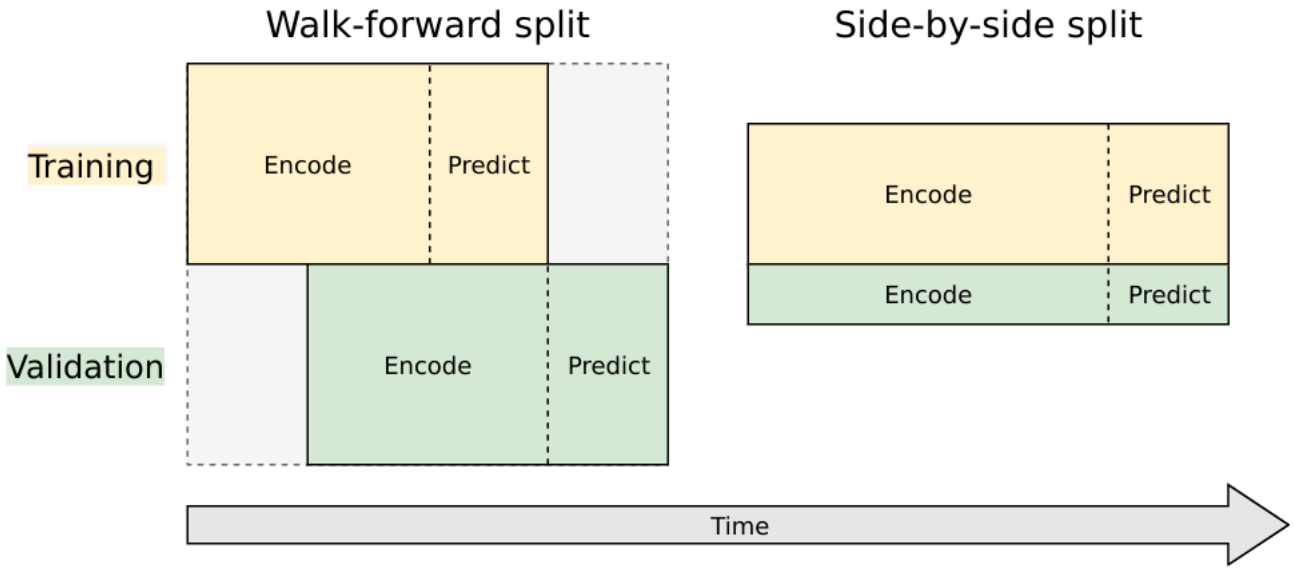
I tried to use RNN activation regularizations from the paper "Regularizing RNNs by Stabilizing Activations", because internal weights in cuDNN GRU can't be directly regularized (or I did not found a right way to do this). Stability loss did'nt worked at all, activation loss gave some very slight improvement for low (1e-06..1e-05) loss weights.

Training and validation

I used COCOB optimizer (see paper Training Deep Networks without Learning Rates Through Coin Betting) for training, in combination with gradient clipping. COCOB tries to predict optimal learning rate for every training step, so I don't have to tune learning rate at all. It also converges considerably faster than traditional momentum-based optimizers, especially on first epochs, allowing me to stop unsuccessful experiments early.

There are two ways to split timeseries into training and validation datasets:

1. *Walk-forward split*. This is not actually a split: we train on full dataset and validate on full dataset, using different timeframes. Timeframe for validation is shifted forward by one prediction interval relative to timeframe for training.
2. *Side-by-side split*. This is traditional split model for mainstream machine learning. Dataset splits into independent parts, one part used strictly for training and another part used strictly for validation.



I tried both ways.

Walk-forward is preferable, because it directly relates to the competition goal: predict future values using historical values. But this split consumes datapoints at the end of timeseries, thus making hard to train model to precisely predict the future.

Let's explain: for example, we have 300 days of historical data and want to predict next 100 days. If we choose walk-forward split, we'll have to use first 100 days for real training, next 100 days for training-mode prediction (run decoder and calculate losses), next 100 days for validation and next 100 days for actual prediction of future values. So we actually can use only 1/3 of available datapoints for training and will have 200 days gap between last training datapoint and first prediction datapoint. That's too much, because prediction quality falls exponentially as we move away from a training data (uncertainty grows). Model trained with a 100 days gap (instead of 200) would have considerable better quality.

Side-by-side split is more economical, as it don't consumes datapoints at the end. That was a good news. Now the bad news: for our data, model performance on validation dataset is strongly correlated to performance on training dataset, and almost uncorrelated to the actual model performance in a future. In other words, side-by-side split is useless for our problem, it just duplicates model loss observed on training data.

Resume?

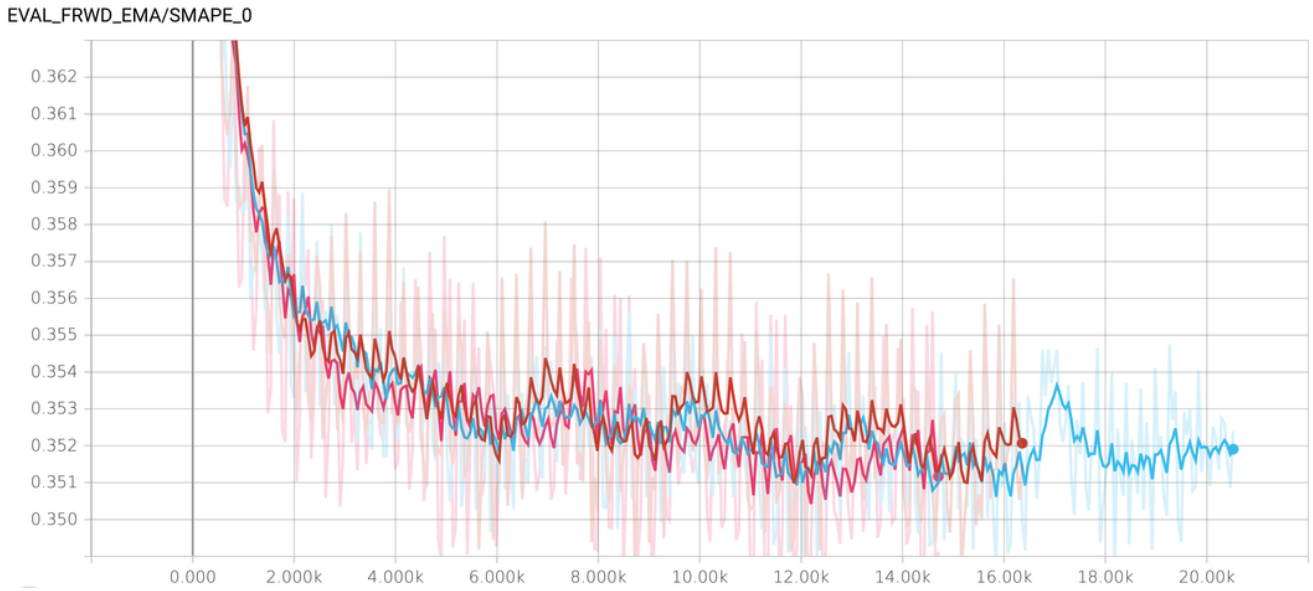
I used validation (with walk-forward split) only for model tuning. Final model to predict future values was trained in blind mode, without any validation.

Reducing model variance

Model has inevitably high variance due to very noisy input data. To be fair, I was surprised that RNN learns something at all on such noisy inputs.

Same model trained on different seeds can have different performance, sometimes model even diverges on "unfortunate" seeds. During training, performance also wildly fluctuates from step to

step. I can't just rely on pure luck (be on right seed and stop on right training step) to win the competition, so I had to take actions to reduce variance.



1. I don't know which training step would be best for predicting the future (validation result on current data is very weakly correlated with a result on a future data), so I can't use early stopping. But I know approximate region where model is (possibly) trained well enough, but (possibly) not started to overfit. I decided to set this optimal region bounds to 10500..11500 training steps and save 10 checkpoints from each 100th step in this region.
2. Similarly, I decided to train 3 models on different seeds and save checkpoints from each model. So I have 30 checkpoints total.
3. One widely known method for reducing variance and improving model performance is SGD averaging (ASGD). Method is very simple and well supported in Tensorflow - we have to maintain moving averages of network weights during training and use these averaged weights, instead of original ones, during inference.

Combination of all three methods (average predictions from 30 checkpoints using averaged model weights in each checkpoint) worked well, I got roughly the same SMAPE error on leaderboard (for future data) as for validation on historical data.

Theoretically, one can also consider two first methods as a kind of ensemble learning, that's right, but I used them mainly for variance reduction.

Hyperparameter tuning

There are many model parameters (number of layers, layer depths, activation functions, dropout coefficents, etc) that can be (and should be) tuned to achieve optimal model performance. Manual tuning is tedious and time-consuming process, so I decided to automate it and use SMAC3 package for hyperparameter search.

Some benefits of SMAC3:

- Support for conditional parameters (e.g. jointly tune number of layers and dropout for each layer; dropout on second layer will be tuned only if n_layers > 1)
- Explicit handling of model variance. SMAC trains several instances of each model on different seeds, and compares models only if instances were trained on same seed. One model wins if it's better than another model on all equal seeds.

Contrary to my expectations, hyperparamter search did not found well-defined global minima. All best models had roughly the same performance, but different parameters. Probably RNN model is too expressive for this task, and best model score depends more on the data signal-to-noise ratio than on the model architecture.

Anyway, best parameters sets can be found in `hparams.py` file

Roberto Spad... • 2 months ago • Options • Reply 1

Hi guys, one doubt... When you have an arima model you can predict E() and E^2(), how could we include an E^2() to this model? In other words, if we predict t=10 what's the E^2() associated with that valie? Any idea?

Arthur Suil... • (1st in this Competition) • 2 months ago • Options • Reply 0

What is E^2? Variance?

Roberto Sp... • 2 months ago • Options • Reply 1

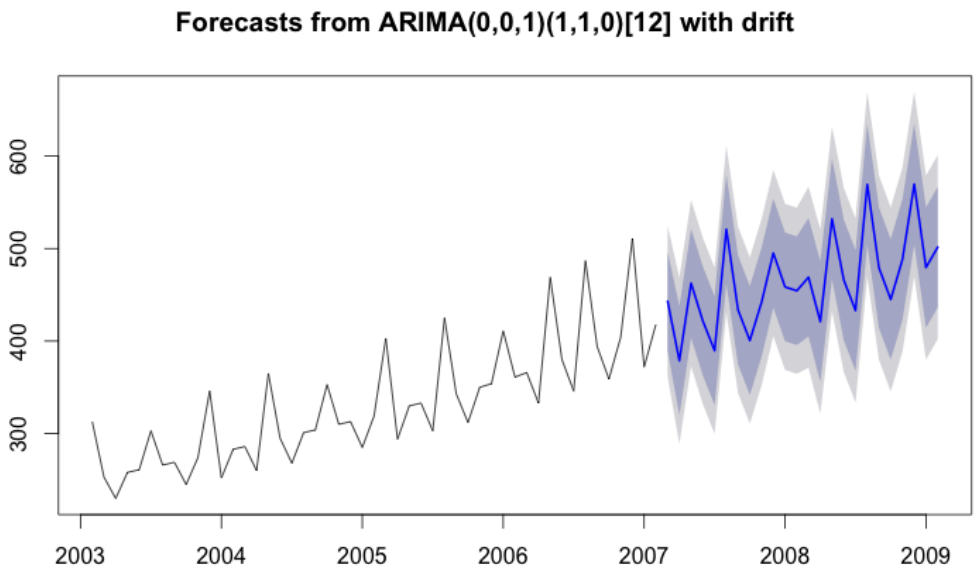
hum i will try to reformulate the question

It's about forecast intervals with ARIMA models (https://en.wikipedia.org/wiki/Autoregressive_integrated_moving_average#Forecast_intervals), but for ARIMA there's an important assumption, "residuals are uncorrelated and normally distributed", to use forecast intervals you check this (shapiro or any other white noise test on residual (error)), but what about others models like NN or when residual isn't white noise or if noise is correlated?

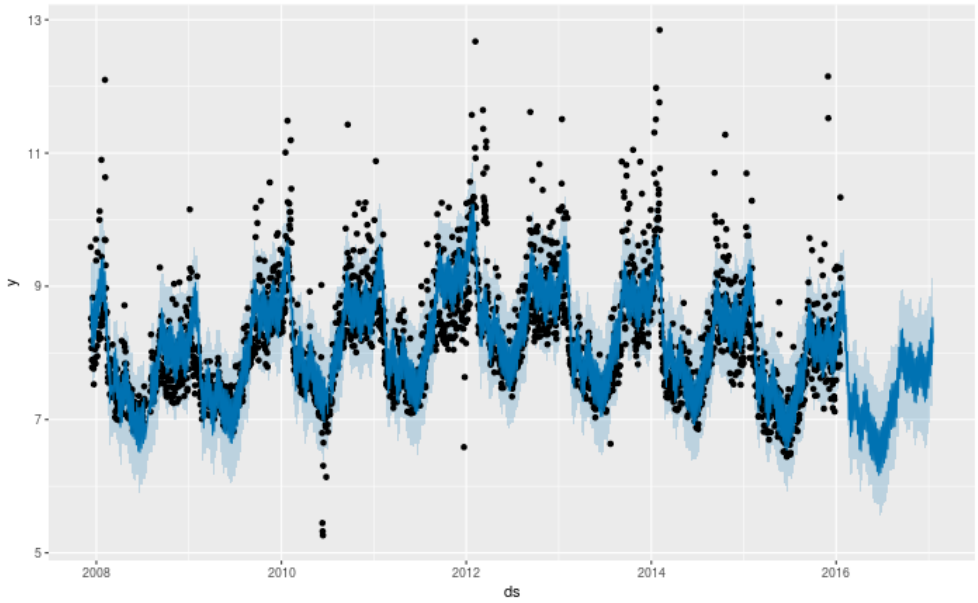
In other words the question is "could be possible to output forecast interval to NN models?". My first idea is include an ŷ2 as variance of y, and train two variables instead of only one, but I'm not sure if it's ok or if an GARCH(1,1) (or rolling variance) over ŷ could work as good forecast interval estimator (it's relative to ŷ and not to error (y-ŷ)), this one was my second idea since we have ŷ values and don't need to retrain the model to include an ŷ2.

I don't know if sounds like crazy or wrong idea about something that already exists.

example of arima interval:



example of prophet interval:



Arthur Suil... • (1st in this Competition) • 2 months ago • Options • Reply 1

It's possible, implementation depends on how you want to model posterior distribution. In a simplest case, we can assume Gaussian distribution, and predict not only mu (as current model does), but pair (mu, sigma). Loss will be negative log probability of data given predicted mu and sigma. In other words, we can treat NN as MLE estimator.

Roberto Sp... • 2 months ago • Options • Reply 1

"predict not only mu (as current model does), but pair (mu, sigma). ", that was my initial idea, but i'm not sure what y_sigma_true should be used, reading you comment "how you want to model posterior distribution", probably that's a question to be answered like error metric... 1)y_sigma_true = garch, rolling std, etc and 2) what metric to optimize, since we have 2y_true (y/sigma)

i'm not sure what metric could be used to optimize, you told MLE, maybe it could be used?

my initial idea was an mse or anything like it, just not sure if 2 y could be optimized at same time to different values (sigma $\simeq y^2$ and y)

(thanks in advance)

Arthur Suil... • (1st in this Competition) • 2 months ago • Options • Reply 1

Let's explain in steps:

1. Predict `mu_hat` , `sigma_hat` for each timeseries step
2. Calculate likelihood `P(data|mu_hat, sigma_hat)` for each step. This is `Normal.pdf(true_pageviews, mu_hat, sigma_hat)` in our case
3. Take log of probability values and average across all steps: `mean(log(p_i))` . This is average log-likelihood of our data for predicted `mu_hat_i` , `sigma_hat_i` . The more accurate our estimations of mu and sigma, the greater the likelihood.
4. Use this loglikelihood as a loss metric for SGD. (use negative loglikelihood, if optimizer wants to minimize the loss).
5. Profit

No need to use garch, rolling std or anything fancy.

Roberto Sp... • 2 months ago • Options • Reply 1

uhmm =) nice, but some doubts yet

> **Arthur Suilin wrote**
>
> > Let's explain in steps:

1. Predict `mu_hat` , `sigma_hat` for each timeseries step

ok, using any model (in our case, your NN)

1. Calculate likelihood `P(data|mu_hat, sigma_hat)` for each step. This is `Normal.pdf(true_pageviews, mu_hat, sigma_hat)` in our case

P(data|mu_hdat,sigma_hat), could be rewrite as "Normal.pdf(true_pageviews, mu_hat, sigma_hat)", i didn't understood it at 'low level'

you have a 'prediction' (y_hat≃mu_hat, sigma_hat) for each 'row', and use it to calculate an "Z score"/normal distribuition probability given the y_true values?

1. Take log of probability values and average across all steps: `mean(log(p_i))` . This is average log-likelihood of our data for predicted `mu_hat_i` , `sigma_hat_i` . The more accurate our estimations of mu and sigma, the greater the likelihood.
2. Use this loglikelihood as a loss metric for SGD. (use negative loglikelihood, if optimizer wants to minimize the loss).

these steps need 2 :P but ok, having mean(log(p())) just minimize and you are done

1. Profit

haha no profit just knowledge here :)

No need to use garch, rolling std or anything fancy.

hum, but what sigma you use at train(x,y) when y=[y,sigma]?

Arthur Suil... • (1st in this Competition) • 2 months ago • Options • Reply 1

You can interpret same probability `P(data|theta)` in two ways:

1. Probability to observe data given parameters `theta` (so probability is a function of data). This is usual 'probability' definition.
2. Likelihood of parameters `theta` given observed data.

You can see details at https://www.quora.com/What-is-the-difference-between-probability-and-likelihood-1/answer/Jason-Eisner

We use second interpretation. Given our pageviews, we calculate how well distribution with `(mu, sigma)` parameters will fit our pageviews. This is absolutely same calculation as probability to see expected number of pageviews given the `(mu, sigma)` distribution parameters. Do you understand this?

> you have a 'prediction' (y_hat≃mu_hat, sigma_hat)

No. `mu_hat` , `sigma_hat` is our prediction. We don't need to calculate `y_hat` (to be precise, it is already calculated: `y_hat` is equivalent to `mu_hat` for Gaussian distribution). We need just to check how well our predicted distribution will fit our data, i.e. check how well this condition holds: `y_true≃Normal(mu_hat, sigma_hat)` . If we have ideal fit, we'll have `y_true=mu_hat` , so peak of predicted Gaussian distribution will be equal to `y_true` value. If we'll have less than ideal fit, `y_true` will be off peak. Likelihood is a measure of our 'fitness'.

> but what sigma you use at train(x,y) when y=[y,sigma]?

Again, we don't need `sigma` at training data. We have only to predict it and compare resulting distribution with `y_true` (calculate likelihood)

Roberto Sp... • 2 months ago • Options • Reply 1

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> We use second interpretation. Given our pageviews, we calculate how well distribution with `(mu, sigma)` parameters will fit our pageviews. This is absolutely same calculation as probability to see expected number of pageviews given the `(mu, sigma)` distribution parameters. Do you understand this?

nice :) some points to understand yet, but you put a pause in the right place haha :D thanks

1) the "P(data|theta)" is calculated as empirical "sum(Yi) / count(Y)", or you consider a distribuition to data/theta (P(data|theta) ≃ N(mu,sigma)), or you consider it as a function that given theta values, return a probability to data?

2) "pageviews" ≃ Y values and X values to estimator, in this case we only consider Y as 'data' (P(data)) and X as theta (P(data|theta)), right?

3) "we calculate how well distribution with `(mu, sigma)` parameters will fit our pageviews", something like reduce error of fitting changing mu/sigma to fit Y ≃ N(mu,sigma)?

> you have a 'prediction' (y_hat≃mu_hat, sigma_hat)

> No. `mu_hat`, `sigma_hat` is our prediction. We don't need to calculate `y_hat` (to be precise, it is already calculated: `y_hat` is equivalent to `mu_hat` for Gaussian distribution).

pause :) in this model (NN you submitted to kaggle) you don't consider the y_hat distribuition, you just want to optimize the smape metric right? the gaussian distribuition isn't important, we are talking about gaussian an mu/sigma just to create a "forecast inteval", right? in this case considering that we force the mu_hat to be gaussian distribuition, we have a well defined sigma_hat that's why we minimize the error of Y≃N(sigma,mu) instead of minimize the smape loss

> We need just to check how well our predicted distribution will fit our data, i.e. check how well this condition holds: `y_true≃Normal(mu_hat, sigma_hat)`. If we have ideal fit, we'll have `y_true=mu_hat`, so peak of predicted Gaussian distribution will be equal to `y_true` value. If we'll have less than ideal fit, `y_true` will be off peak. Likelihood is a measure of our 'fitness'.
>
> > but what sigma you use at train(x,y) when y=[y,sigma]?
>
> Again, we don't need `sigma` at training data. We have only to predict it and compare resulting distribution with `y_true` (calculate likelihood)

nice like somelines up, you don't need cause you force a gaussian distribution, right? :)

if i'm right... considering that optimizing smape (and not the fit of gaussian distribuition) we couldn't estimate the probability distribuition of the kaggle submition y_hat values? for example at day 20 model output y_hat=30, but what probability of 30 being right or not? (when you optimize you just optimize the smape error, and you will have a model that output the 'more probable value for minimal smape error, instead of probability distribuitions', in other words, when you fit using smape, you couldn't output a probability density to that point being predicted, only if you force a well known distribuition (gaussian in our case of mu/sigma), or you can?

that's a nice discussion, thanks anyway if we don't converge, I never asked something like this to teachers at university/mba/school =)

Arthur Suil... • (1st in this Competition) • 2 months ago • Options • Reply 0

> in this model (NN you submitted to kaggle) you don't consider the y_hat distribuition, you just want to optimize the smape metric right? the gaussian distribuition isn't important, we are talking about gaussian an mu/sigma just to create a "forecast inteval", right? in this case considering that we force the mu_hat to be gaussian distribuition, we have a well defined sigma_hat that's why we minimize the error of Y≃N(sigma,mu) instead of minimize the smape loss

Right.

> if i'm right... considering that optimizing smape (and not the fit of gaussian distribuition) we couldn't estimate the probability distribuition of the kaggle submition y_hat values?

Right. To learn model to predict confidence interval, we should have a loss that depends on quality of confidence interval prediction. SMAPE knows nothing about confidence, so we can't use it.

So please forget SMAPE and think in terms of distributions and likelihoods. If you switch your mind into 'probabilistic mode' and read some probability/likelihood articles (including the link I gave you), you'll understand the whole picture.

Single Gaussian distribution is a primitive case, where are many advanced ways to model posterior distribution (histogram estimation, kernel density estimation, distribution mixtures), but Gaussian is easiest to understand.

Roberto Sp... • 2 months ago • Options • Reply 2

nice =) i think we already converged

this maybe help to explain why arima/prophet models don't have a high performace as NN optimized to smape loss, arima try to 'convert' every time series to 'white noise error', i don't know about prophet. I think i understood the idea of "think about distributions and likelihoods", you must "select" a distribuition first (or select the distribuition that best fit data) and fit the parameters to have a P() function instead of using "any_ml_model.predict() or predict_proba()" and then you can estimate intervals from cdf/pdf functions, right? :)

going back to y=[y,variance] instead of y=[y]... maybe the idea of y=[y,garch(1,1) or any other variance estimator] could "create" the "interval confidence", or at least a variance associated with that value? the problem should be what metric/loss function to optimize this and if this could be used to estimate the interval, i'm not sure yet if given some model (anyone) we could create a confidence interval. my last idea should be estimating the error² from Y_hat-Y given the output of model, and train a model to predict this, but it'm not sure if this is valid or not, or if there's a technique to do this without knowing the probability being used with the model (sorry if it's out of scope, i'm just thinking about how to have something like arima models with any kind of model)

Arthur Suil... • (1st in this Competition) • 2 months ago • Options • Reply 1

> you must "select" a distribuition first (or select the distribuition that best fit data) and fit the parameters to have a P() function instead of using "any_ml_model.predict() or predict_proba()" and then you can estimate intervals from cdf/pdf functions, right?

Right. You can also use non-parametric models (histograms, kernel density estimators) instead of selecting hardcoded distribution.

> i'm just thinking about how to have something like arima models with any kind of model

RNN is ARIMA on steroids. I can do all that ARIMA can do and much, much more. I really don't see a reasons to work with ARIMA-like models, except of some amount of interpretability.

BTW, ARIMA 'confidence estimation' is really based on dumb assumption of Gaussian distribution (exactly same as we discussed above). I think it's better to use explicit, transparent and controllable distributions instead of hidden assumptions, buried deep in ARIMA or GARCH models.

Roberto Sp... • 2 months ago • Options • Reply 1

> RNN is ARIMA on steroids. I can do all that ARIMA can do and much, much more. I really don't see a reasons to work with ARIMA-like models, except of some amount of interpretability.

yeap :) and some others things that papers report is convolution being something like 'automatic' filtering (fir/irr filters) and max pooling ≃ automatic feature extraction, in this case 1d conv since it's only timeseries (time dimension), 2d to images (x,y), 3d to videos (time,x,y) / medical images (xyz, lung cancer competition ≃ science bowl)

> BTW, ARIMA 'confidence estimation' is really based on dumb assumption of Gaussian distribution (exactly same as we discussed above). I think it's better to use explicit, transparent and controllable distributions instead of hidden assumptions, buried deep in ARIMA or GARCH models.

nice, the idea of creating a second model to predict the error² isn't too crazy =)

very nice discussion =)