

Feature generation for multiscale time series forecasting multimodels

LIG

Technical report (pre-draft)

Notation

$\mathfrak{D} = \{\mathbf{s}^{(m)} m = 1, \dots, M\}$	large set of time series
$\bar{\mathbf{s}}$	special case of time series \mathbf{s} for classification
T_{\max}	maximum number of time stamps
Δt_p	local prehistory
Δt_r	defines time period (requested) for prediction
$\mathbf{s}_i^{(m)} = [\mathbf{y}_i^{(m)} \mathbf{x}_i^{(m)}]$	local (t_i) segment from the time series $\mathbf{s}^{(m)}$
$\mathbf{X}^*, \mathbf{x}_i^* = [\mathbf{y}_i \mathbf{x}_i]$	object-feature matrix, $\mathbf{y}_i = [\mathbf{y}_i^{(1)}, \dots, \mathbf{y}_i^{(M)}]$, $\mathbf{x}_i = [\mathbf{x}_i^{(1)}, \dots, \mathbf{x}_i^{(M)}]$
\mathbf{Y}, \mathbf{X}	target matrix, feature matrix
q	number of objects \mathbf{x}_i^* extracted from \mathfrak{D}
r	dimensionality of the target vector $[\mathbf{y}_i^{(1)}, \dots, \mathbf{y}_i^{(M)}]$
n	dimensionality of the feature vector $[\mathbf{x}_i^{(1)}, \dots, \mathbf{x}_i^{(M)}]$
$\mathbf{x}_0^* = [\mathbf{y}_0 \mathbf{x}_0]$	a testing object?
$\mathcal{J} = 1, \dots, n$	feature index set
$\mathcal{A} \subset \mathcal{J}$	the subset of feature indices
$\mathbf{f}_k(\mathbf{w}_{\mathcal{A}_k}, \mathbf{x}), k = 1, \dots, K$	regression model, defined for a subset \mathcal{A}_k
$\mathbf{w}_{\mathcal{A}_k}$	model parameters (alternatively, \mathbf{w}_k)
$\boldsymbol{\pi} = [\pi_{i1}, \dots, \pi_{iK}]$	vector of correspondence
$\mathcal{I} = \{1, \dots, m\} = \mathcal{B}_0 \sqcup_k \mathcal{B}_k$	set of object indices
\mathcal{B}_0	test set
$\mathcal{B}_k, k = 1, \dots, K$	training sets

Q	quality function
S	error function
$g = g(\mathbf{b}, s)$	parametric functions for feature transformation
$\mathfrak{G} = \{g : \mathbf{s} \rightarrow \phi\}$	set of feature transformations
$\phi = [\phi^1, \dots, \phi^M]$	generated feature vector
$\varepsilon = \mathbf{y} - \hat{\mathbf{y}}$	vector of residuals
$\mathbf{c}_1^1, \dots, \mathbf{c}_P^M$	k -means centroids
\mathbf{H}^*	Hankel matrix
$\theta = [\mathbf{w}_1, \dots, \mathbf{w}_k, \boldsymbol{\pi}, \beta]$	parameters of the mixture model
z_{ik}, γ_{ik}	latent (correspondence) variables and their expectations (mixture models)

1 Introduction

The paper investigates behavior of a device within the concept of Internet of Things. The device at question is monitored by a set of sensors, which produces large amount of multiscale time series during its lifespan. These time series have various time scales since distinct sensor produce measurements with various frequencies (milliseconds, days, weeks, etc). The main goal is to forecast the next state of a device. **What exactly is this state?**

We assume that the sampling rate of each time series is fixed and each time series has its own forecast horizon. Examples of this kind of time series are listed below. **(list)**

Furthermore, the time history is assumed sufficiently long to construct an adequate forecasting model; the time series are assumed to have auto- and cross-correlation dependencies.

In the next Sections we explain how to construct **vector autoregressive models** and test their quality under the listed conditions. TODO (list and review state of the art).

2 Problem statement

Consider a large set of time series $\mathfrak{D} = \{\mathbf{s}^{(m)} \mid m = 1 \dots, M\}$, where each real-valued time series \mathbf{s} has its own sampling rate $f_s^{(m)}$. The sampling rate might be changing over time, or the ratio between different sampling rates might be non-rational. In such cases as well

as for time series with missing values we apply resampling procedure, which is described further.

2.1 Time series resampling

Let the time t be in continuous set \mathbb{R}_+^1 and the time series \mathbf{s} be piece-wise constant. There are three possibilities to create such time series from a discrete-values one: 1) the constant goes after the sample $s(t)$, 2) before the sample, 3) in the neighborhood of the sample. See red, green and blue lines in the Figure 1a.

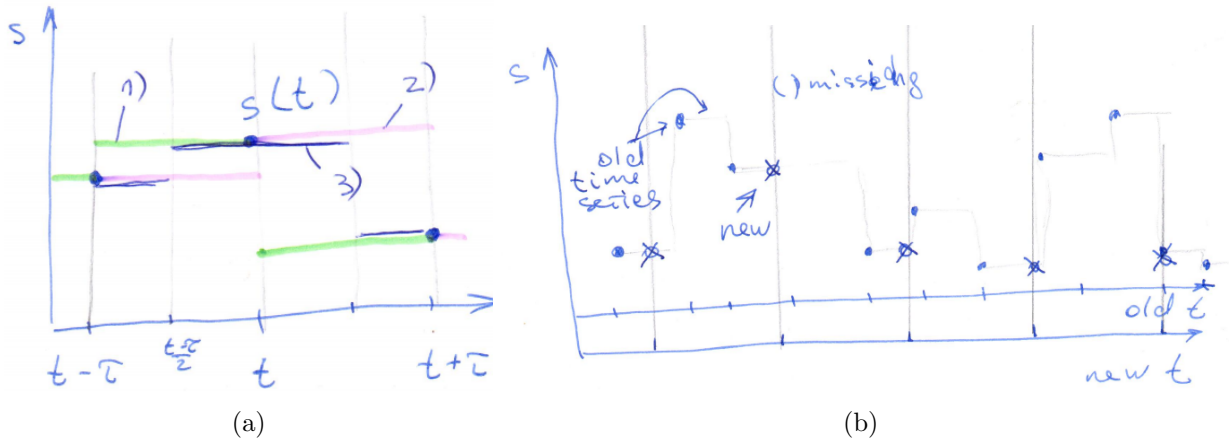


Figure 1: Piece-wise representation of a time series.

This assumptions helps introducing a new sampling rate and eliminates the problem of missing values, since the previous (next, current in the terms of Fig. 1a) value holds continuously until the following comes. The constant model could be developed into more complex one: a piece-wise linear, quadratic or cubic spline with its nodes in the time-ticks or over the time-ticks according to the following criterions: 1) NyquistShannon theorem, 2) Fisher-Neyman theorem. The following optimization problem returns the new sampling rate:

todo

This fixed rate is used to obtain a resampled time series with regular time-ticks.

Selecting sampling rate: NyquistShannon sampling theorem. Suppose that a signal $s(t)$ is bandlimited with frequency f_b . According to the NyquistShannon sampling

theorem, it is sufficient to sample the signal with frequency

$$\frac{1}{T} = f_s > 2f_b \quad (1)$$

to be able to fully reconstruct the signal from its discretely sampled measurements $s(t_i) = s(iT)$. Alternatively, for $f_s > 2f_b$, Whittaker-Shannon interpolation

$$s(t) = \sum_{i=-\infty}^{\infty} s(i \cdot T) \text{sinc} \left(\frac{t - iT}{T} \right)$$

of the time series $s(t_i)$ yields perfect reconstruction of the signal $s(t)$. Sampling with $f_s < 2f_b$ causes distortions known as aliasing. In this case the time series have to be low-pass filtered to satisfy the Nyquist condition (1).

FFT resampling. In signal processing a common way to change resolution of a signal is to use a combination of upsampling and decimation, implemented here via FFT transform and downsampling. Suppose that desired sampling rate f_{rs} is fixed, that is, we would like to approximate $T_{rs} = f_{rs}T_s$ uniformly sampled observations $s(\tilde{t}_i)$, $i = 1, \dots, T_{rs}$ of the time series $s(t_i)$, $i = 1, \dots, T_s$. Let $G_s = \{t_1, \dots, T_s\}$ and $G_{rs} = \{\tilde{t}_1, \dots, T_{rs}\}$ denote the current and the desired grids. The first step to resampling $\mathbf{s}(G_s) \rightarrow \mathbf{s}(G_{rs})$ is the piecewise approximation $\hat{\mathbf{s}} = \mathbf{s}(G_{\text{joint}})$ (see Fig. 1a and Fig. 1b)

$$\hat{s}(\tilde{t}_i) = s(t_i), \text{ where } t_i = \max\{t \in G_s \text{ and } t \leq \tilde{t}_i\}. \quad (2)$$

of \mathbf{s} at $G_{\text{joint}} = G_s \cup G_{rs}$. To increase the smoothness of piecewise approximation $\hat{\mathbf{s}}$ we apply low pass DFT filtering to $\mathbf{s}(G_{\text{joint}})$, so that the reconstructed time series $\mathbf{s}_{\text{lf}}(G_{\text{joint}})$ are bandlimited with $f_b < f_{rs}/2$ and then downsample the output $\mathbf{s}(G_{\text{joint}})$ to G_{rs} .

The cutoff frequency f_b is set so that fixed ratio $1 - \alpha$ of the power spectrum density is preserved:

$$\sum_{Nf_b < k \leq N-1} |S_k|^2 < \alpha \sum_{k=0}^{N-1} |X_k|^2, \quad (3)$$

where X_k are the FFT coefficients of $s(iT)$.

Selecting sampling rate: Fisher-Neyman resampling criterion. TODO

Algorithm 1: FFT rescaling procedure.

TimeSeriesRescaling()

begin

Data: time series $\mathbf{s}(G_s)$, sampled at $G_s = \{t_1, \dots, T_s\}$.

Parameters: desired grid $G_{rs} = \{\tilde{t}_1, \dots, T_{rs}\}$.

Result: resampled time series $\mathbf{s}(G_{rs}) = \{\tilde{s}(\tilde{t}_i) | i \in G_{rs}\}$.

 Form the new grid $G_{\text{joint}} = G_s \cup G_{rs}$

 Upsample time series, using piecewise approximation:

$\hat{\mathbf{s}} = \mathbf{Piecewise}(\mathbf{s}, G_s, G_{rs})$

 Apply low pass filtering $\hat{\mathbf{s}}$:

$\hat{\mathbf{s}}_{\text{lf}} = \mathbf{LowPassFFTFiltering}(\hat{\mathbf{s}}, \frac{f_s}{2} - \varepsilon)$

 Downsample $\hat{\mathbf{s}}_{\text{lf}}$ to \tilde{G} :

$\tilde{\mathbf{s}} = [\hat{s}_{\text{lf}}(\tilde{t}_1), \dots], \tilde{t}_i \in \tilde{G}$.

Piecewise()

begin

Data: Time series, \mathbf{s} . **Parameters:** original grid G , new grid \tilde{G} .

Result: Upsampled time series $\hat{\mathbf{s}} = \{\hat{s}(\hat{t}_i) \in G \cup \tilde{G}\}$.

 Form new grid $\hat{G} = G \cup \tilde{G}$: $\hat{G} = \{\hat{t}_1 < \dots < \hat{t}_i < \dots < T_s | \hat{t}_i \in G \cup \tilde{G}\}$

 For each $\hat{t}_i \in \hat{G}$: **if** $\hat{t}_i \in G$: **then**

$\hat{s}(\hat{t}_i) = x(\hat{t}_i)$

else

$\hat{s}(\hat{t}_i) = x(t_i)$, where $t_i = \max\{t : t \in G \text{ and } t < \hat{t}_i.\}$

LowPassFFTFiltering()

begin

Data: Time series, \mathbf{s} . **Parameters:** cut-off value f_b for high frequencies.

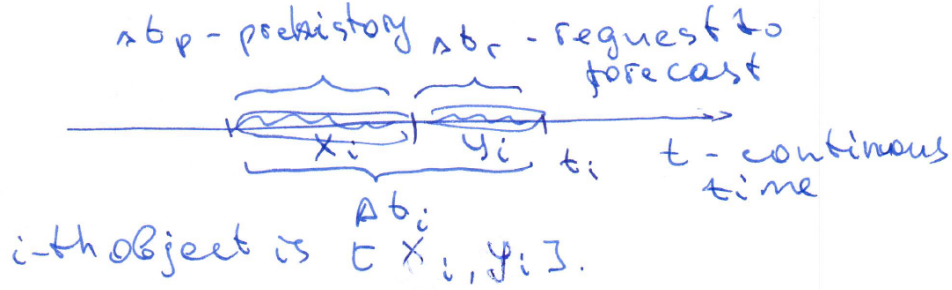
Result: Filtered time series $\tilde{\mathbf{s}}_{\text{lf}}$.

 Zero-pad \mathbf{s} , so that $|\mathbf{s}| = 2^N$, where $N = \lceil \log_2(|\mathbf{s}|) \rceil$

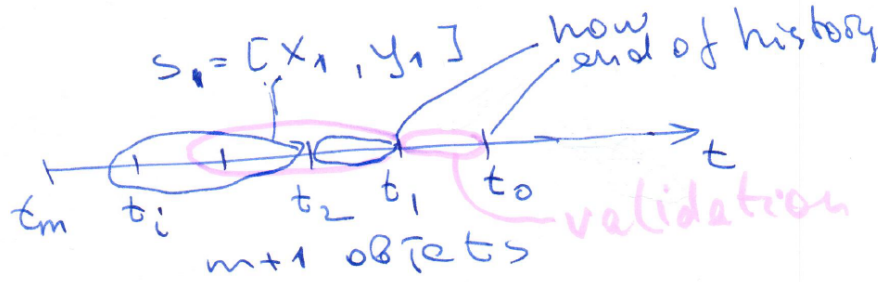
 Find FFT coefficients a_j, b_j for $j = 1, \dots, N$ for \mathbf{s}

 Set $a_j = 0, b_j = 0$, for $2\pi w_j > f_b$

 Reconstruct the time series, using inverse FFT.



(a)



(b)

Figure 3: Draw an object from time series history.

constructed as follows (Fig. 3b). Let $\mathbf{s}_i^{(m)}$ denote the i -th segment of the time series $\mathbf{s}^{(m)}$

$$\mathbf{s}_i^{(m)} = [\mathbf{y}_i^{(m)} | \mathbf{x}_i^{(m)}] = [\underbrace{s^{(m)}(t_i), \dots, s^{(m)}(t_i - \Delta t_r)}_{\mathbf{y}_i^{(m)}}, \underbrace{s^{(m)}(t_i - \Delta t_r - \Delta t_p)}_{\mathbf{x}_i^{(m)}}], \quad (4)$$

where $s^{(m)}(t)$ is an element of time series $\mathbf{s}^{(m)}$. Select $t_i, i = 1, \dots, q$ from $G_s = \{1, \dots, T_{\max}\}$ so that vectors $\mathbf{s}_i = [\mathbf{y}_i, \mathbf{x}_i]$ cover time series \mathbf{s}

$$\{s(1), \dots, s(T_{\max})\} = \bigcup_{i=1}^{q-1} \{s(t_i - \Delta t_r), \dots, s(t_i)\} \quad (5)$$

with overlap in feature parts \mathbf{x}_i and no intersection in target parts \mathbf{y}_i :

$$|t_{i+1} - t_i| > \Delta t_r.$$

Following (4) and (5), extract segments $i = 1, \dots, q$ from all time series $\mathbf{s}^{(m)} \in \mathfrak{D}$ and form

the matrix

$$\mathbf{X}^* = \left[\begin{array}{ccc|ccc} \mathbf{y}^{(1)} & \dots & \mathbf{y}^{(M)} & \mathbf{x}_0^{(1)} & \dots & \mathbf{x}_0^{(M)} \\ \mathbf{y}_1^{(1)} & \dots & \mathbf{y}_1^{(M)} & \mathbf{x}_1^{(1)} & \dots & \mathbf{x}_1^{(M)} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\ \mathbf{y}_q^{(1)} & \dots & \mathbf{y}_q^{(M)} & \mathbf{x}_q^{(1)} & \dots & \mathbf{x}_q^{(M)} \end{array} \right] = \left[\begin{array}{c|c} \mathbf{y}_0 & \mathbf{x}_0 \\ \hline \mathbf{Y} & \mathbf{X} \end{array} \right]_{\substack{1 \times r \\ q \times r} \quad \substack{1 \times n \\ q \times n}}.$$

Denote a row from the pair \mathbf{Y}, \mathbf{X} as \mathbf{y}, \mathbf{x} and call these vectors the target and the features.

Feature selection and multimodelling. As one must forecast all elements from the target \mathbf{y} , only a few elements from the features \mathbf{x} are supposed to be informative in terms of the forecast quality. Denote the index set $\mathcal{J} = \{1, \dots, n\}$ and select the subset of the indexes $\mathcal{A} \in \mathcal{J}$. Introduce the forecasting model

$$\hat{\mathbf{y}}_i = \sum_{k=1}^K \pi_{ik} \mathbf{f}_k(\mathbf{w}_{\mathcal{A}_k}, \mathbf{x}_{i, \mathcal{A}_k})$$

as some linear combination of K models and call it the *multimodel*. Each model \mathbf{f}_k has its parameters \mathbf{w}_k and selected features $\mathbf{x}_{\mathcal{A}_k}$. The coefficient π_{ik} set a vector \mathbf{x}_i in correspondence to the model \mathbf{f}_k , so that

$$\sum_{k=1}^K \pi_{ik} = 1 \quad \text{for } i \in \mathcal{I} = \{1, \dots, m\}$$

with two options are to be considered: $\pi \in \{0, 1\}$ and $\pi \in [0, 1]$. Let the forecasting error be

$$S = \sum_{i \in \mathcal{B}_0} \|\hat{\mathbf{y}}_i - \mathbf{y}_i\|_1,$$

where the set of object indexes \mathcal{I} is splitted to the test set \mathcal{B}_0 and the train sets,

$$\mathcal{I} = \mathcal{B}_0 \sqcup_{k=1}^K \mathcal{B}_k.$$

State the forecasting problem as a problem to minimize the error function S given models $\mathbf{f}_1, \dots, \mathbf{f}_K$ by optimizing matrix $\Pi = [\pi_{ik}]$, finite sets $\mathcal{A}_1, \dots, \mathcal{A}_K$ and model parameters $\mathbf{w}_1, \dots, \mathbf{w}_K$ on the sample set with indexes $\mathcal{I} \setminus \mathcal{B}_0$.

2.3 Special case of the problem

A special case of the problem is an early warning forecasting. There is a special time series \bar{s} with its elements $\bar{s} \in \{0, 1\}$. Here zero is interpreted as a *normal state* of the system and one means the system goes from normal to the *abnormal* state without return over time t . The problem is to maximize the lapse of the time segment

$$\|\Delta t_r\| \rightarrow \max,$$

where the vector

$$[\mathbf{y}_0, \mathbf{x}_0] = [0, \dots, 0, 0, \dots, 0, 1],$$

which means the system was in the normal state before it changes. Since the quality Q of forecasting time series \bar{s} depends on $\|\Delta t_r\|$ (the letter time lapse before the warning the higher the forecasting quality [ref]) the minimum level of quality must be set. Let the minimum forecasting quality be

$$Q \{(\hat{\mathbf{y}}_i, \bar{\mathbf{y}}_i) \mid i \in \mathcal{B}_0\} = \text{AUC} = Q_{\text{req}}.$$

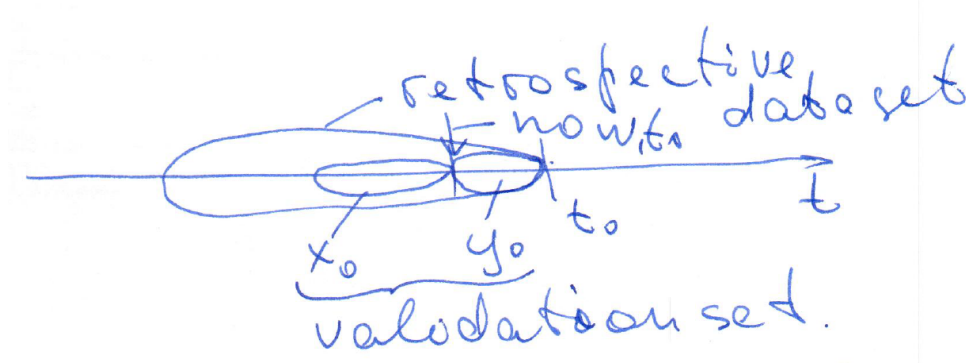


Figure 4: Retrospective forecast includes most recent samples in data set.

Forecast analysis. We consider the forecast testing procedure, given by the algorithm 2. Since our ultimate goal is to construct a forecasting model \mathbf{f} be able to obtain forecasts $\hat{\mathbf{y}}_i$ at any given time $t \leq t_i + \Delta t_r$ we have to imitate this setting, using the so-called retrospective forecast 4 (rolling forecasts, walking ahead predictions). Here we conceal most recent historical samples \mathbf{x}_0^* and make predictions as if they were unknown. Then the quality of the model \mathbf{f} is evaluated according to its performance on these concealed samples.

Forecasting errors. Hyndman [1] divides forecasting errors into four types:

- scale-dependent metrics, such as mean absolute error

$$MAE = \frac{1}{r} \sum_{i=1}^r |\varepsilon_i|,$$

- percentage-error metrics such as the mean absolute percent error

$$MAPE = \frac{1}{r} \sum_{i=1}^r \frac{|\varepsilon_i|}{|y_0(i)|},$$

or symmetric MAPE

$$sMAPE = \frac{1}{r} \sum_{i=1}^r \frac{2|\varepsilon_i|}{|\hat{y}_0(i) + y_0(i)|},$$

- relative-error metrics, measure the average ratio of the errors from a designed method to the errors ε^* of a benchmark method

$$MRAE = \frac{1}{r} \sum_{i=1}^r \frac{|\varepsilon_i|}{\varepsilon_i^*},$$

- and scale-free error metrics, which express each error as a ratio to an average error from a baseline method:

$$MASE = \frac{n-1}{r} \frac{\sum_{i=1}^r |\varepsilon_i|}{\sum_{j=2}^n |x_0(j) - x_0(j-1)|}.$$

3 Feature generation

List of procedures for constructing the feature and the object sets will be placed here.

Discussion point: vector **y** **remains always unchanged**.

The feature set $\mathcal{J} = \bigcup_k \mathcal{A}_k$ includes

- 1) the local history of all time series themselves,
- 2) transformations (non-parametric and parametric) of local history,
- 3) parameters of the local models,
- 4) distances to the centroids of local clusters.

Algorithm 2: Train-test split.

ComputeForecastingErrors()

begin

Data: $\mathbf{X}^* \in \mathbb{R}^{M \times (\Delta t_r + \Delta t_p)}$. Parameters: sample size m , train to test ratio α .

Result: Forecasting quality: root-mean-squared error.

while $n \leq M - m$: **do**

define, $\mathbf{X}_n^* = [\mathbf{x}_n^*, \dots, \mathbf{x}_{m+n-1}^*]^\top$

$\mathbf{X}_{\text{train}}, \mathbf{X}_{\text{test}}, \mathbf{X}_{\text{val}} = \text{TrainTestSplit}(\mathbf{X}_n^*, \alpha)$

train forecasting model $\mathbf{f}(\mathbf{x}, \hat{\mathbf{w}}_n)$, using $\mathbf{X}_{\text{train}}$ and \mathbf{X}_{test}

obtain vector of residuals $\boldsymbol{\varepsilon} = [\varepsilon_T, \dots, \varepsilon_{T-\Delta t_r+1}]$ with respect to \mathbf{X}_{val}

compute forecasting quality:

$$\text{MAPE}(n) = \sqrt{\frac{1}{\Delta t_r} \sum_{t=0}^{\Delta t_r} \varepsilon_{T-t}^2}$$

$n = n + 1$

(or any adequate error function from 2.3)

Average MAPE (other error) by data splits.

TrainTestSplit()

begin

Data: Object-feature matrix $\mathbf{X}^* \in \mathbb{R}^{m \times (\Delta t_r + \Delta t_p)}$. Train to test ratio α .

Result: Train, test, validation matrices $\mathbf{X}_{\text{train}}^*, \mathbf{X}_{\text{test}}^*, \mathbf{X}_{\text{val}}^*$.

Set train set and test set sizes:

$$m_{\text{train}} = \lfloor \alpha(m - 1) \rfloor$$

$$m_{\text{test}} = m - 1 - m_{\text{train}}$$

Decompose matrix \mathbf{X}^* into train, test, validation matrices $\mathbf{X}_{\text{train}}^*, \mathbf{X}_{\text{test}}^*, \mathbf{X}_{\text{val}}^*$:

$$\mathbf{X}_{\text{train}}^* = \left[\begin{array}{c} \mathbf{x}_{\text{val}}^* \in \mathbb{R}^{1 \times (\Delta t_r + \Delta t_p)} \\ \mathbf{X}_{m_{\text{test}}}^* \in \mathbb{R}^{m_{\text{test}} \times (\Delta t_r + \Delta t_p)} \\ \mathbf{X}_{m_{\text{train}}}^* \in \mathbb{R}^{m_{\text{train}} \times (\Delta t_r + \Delta t_p)} \end{array} \right] = \left[\begin{array}{c|c} \mathbf{y}_{\text{val}} & \mathbf{x}_{\text{val}} \\ \mathbf{Y}_{m_{\text{test}}} & \mathbf{X}_{m_{\text{test}}} \\ \mathbf{Y}_{m_{\text{train}}} & \mathbf{X}_{m_{\text{train}}} \end{array} \right]$$

The object set $\mathcal{I} = \sqcup_k \mathcal{B}_k$ includes

- 1) the local history,
- 2) parametric local models and their residuals (including ones from previous iterations),
- 3) DTW-shifted local history as a local forecasting procedure,
- 4) aggregated subsets of time series.

Denote the generated feature vector as ϕ . This vector consists of concatenated row-vectors $\phi = [\phi^{(1)}, \dots, \phi^{(M)}]$, which corresponds to time series local histories $\mathbf{s} = [\mathbf{s}^{(1)}, \dots, \mathbf{s}^{(M)}]$, modified with set of transformations \mathfrak{G} . The elements $g : \mathbf{s} \rightarrow \phi$ of this set are listed below.

3.1 Transformations of local history

The tables 2, 3, 4, 5, 6 list the time series transformation functions. There are non-parametric and parametric procedures to generate features. For the parametric functions $g = g(\mathbf{b}, \mathbf{s})$ the default values of the parameters \mathbf{b} are assigned empirically.

The parametric procedure request two optimization problem statements of the model parameters \mathbf{w} and the primitive function parameters \mathbf{b} . The first one fixes the vector $\hat{\mathbf{b}}$, collected over all the primitive functions $\{g\}$, which generate features ϕ :

$$\hat{\mathbf{w}} = \arg \min S(\mathbf{w} | \mathbf{f}(\mathbf{w}, \mathbf{x}), \mathbf{y}), \quad \text{where} \quad [\mathbf{y}, \mathbf{x}] = \phi(\hat{\mathbf{b}}, \mathbf{s}).$$

The second one optimizes the transformation parameters $\hat{\mathbf{b}}$ given obtained model parameters \mathbf{w}

$$\hat{\mathbf{b}} = \arg \min S(\mathbf{b} | \mathbf{f}(\hat{\mathbf{w}}, \mathbf{x}), \mathbf{y}).$$

This procedure repeats two problems until vectors $\hat{\mathbf{w}}, \hat{\mathbf{b}}$ converge. The initial values of vector \mathbf{b} (are shown in table ??). Due to the various origins of the time series and their transformations the residual vector should be normalized:

$$\epsilon = \frac{\hat{\mathbf{y}} - \mathbf{y}}{|\mathbf{y}| \cdot \|\mathbf{y}\|_2^1}.$$

It (transformation? normalization) does not change the number elements in the vectors, $|\phi| = |\mathbf{s}|$.

3.2 Convolutions, statistics and parameters of local history

The listed feature generation functions convolves time series, so they reduce the dimensionality $|\phi = \mathbf{g}(\mathbf{s})| < |\mathbf{s}|$.

3.3 Parameters of local history forecast

For the time series \mathbf{s} construct the Hankel matrix with a period k and shift p , so that for $\mathbf{s} = [s_1, \dots, s_T]$ the matrix

$$\mathbf{H}^* = \left[\begin{array}{c|cc} s_T & \dots & s_{T-k+1} \\ \vdots & \ddots & \vdots \\ s_{k+p} & \dots & s_{1+p} \\ s_k & \dots & s_1 \end{array} \right], \text{ where } 1 \geq p \geq k.$$

Reconstruct the regression to the first column of the matrix $\mathbf{H}^* = [\mathbf{h}, \mathbf{H}]$ and denote its least square parameters as the feature vector

$$\boldsymbol{\phi}^{(m)} = \arg \min \|\mathbf{h} - \mathbf{H}\boldsymbol{\phi}\|_2^2.$$

For the time series $\mathbf{s}^{(m)}$, $m = 1, \dots, M$ use the parameters $\boldsymbol{\phi}^{(m)}$ as the features.

3.4 Distances to centroids of local clusters

This procedure applies the kernel trick to the time series. For given local history time series $\mathbf{x}_i^{(m)}$, $m = 1, \dots, M$ compute k -means centroids $\mathbf{c}_p^{(m)}$, $p = 1, \dots, P$. With the selected k -means distance function ρ construct the feature vector

$$\boldsymbol{\phi}_i^{(m)} = [\rho(\mathbf{c}_1^{(m)}, \mathbf{s}_i^{(m)}), \dots, \rho(\mathbf{c}_P^{(m)}, \mathbf{s}_i^{(m)})] \in \mathbb{R}_+^P.$$

This k -means of another clustering procedure may use internal parameters, so that there are no parameters to be included to the feature vector or to the forecasting model.

4 Feature selection

TODO

5 Mixture models

Let $D = (X, \mathbf{y})$ denote the data, where $X = [\mathbf{x}_1^\top, \dots, \mathbf{x}_i, \dots, \mathbf{x}_m^\top]^\top$, denotes the inputs $\mathbf{x}_i \in \mathbb{R}^n$, \mathbf{y} denotes the targets $y_i \in Y$. The task is to estimate y_i , given \mathbf{x}_i . Assuming

Table 2: Must-try functions.

Formula	Output dimension	# of arguments	# of parameters
\sqrt{x}	1	1	0
$x\sqrt{x}$	1	1	0
$\arctan x$	1	1	0
$\ln x$	1	1	0
$x \ln x$	1	1	0

Table 3: List of elementary functions.

Function name	Formula	Output dimension	# of arguments	# of parameters
Add constant	$x + w$	1	1	1
Quadratic	$w_2x^2 + w_1x + w_0$	1	1	3
Cubic	$w_3x^3 + w_2x^2 + w_1x + w_0$	1	1	4
Logarithmic sigmoid	$1/(w_0 + \exp(-w_1x))$	1	1	2
Exponent	$\exp x$	1	1	0
Normal	$\frac{1}{w_1\sqrt{2\pi}} \exp\left(\frac{(x-w_2)^2}{2w_1^2}\right)$	1	1	2
Multiply by constant	$x \cdot w$	1	1	1
Monomial	$w_1x^{w_2}$	1	1	2
Weibull-2	$w_1w_2x^{w_2-1} \exp -w_1x^{w_2}$	1	1	2
Weibull-3	$w_1w_2x^{w_2-1} \exp -w_1(x - w_3)^{w_2}$	1	1	3

linear model f with gaussian noise

$$y = f(\mathbf{x}, \mathbf{w}) + \varepsilon, \quad f(\mathbf{x}, \mathbf{w}) = \mathbf{w}^\top \mathbf{x}, \quad \varepsilon \sim \mathcal{N}(0, \beta) \Rightarrow y \sim \mathcal{N}(\mathbf{w}^\top \mathbf{x}, \beta),$$

Table 4: Monotone functions.

By growth rate					
Function name	Formula	Output dimension	# of arguments	# of parameters	Constraints
Linear	$w_1x + w_0$	1	1	2	
Exponential rate	$\exp(w_1x + w_0)$	1	1	2	$w_1 > 0$
Polynomial rate	$\exp(w_1 \ln x + w_0)$	1	1	2	$w_1 > 1$
Sublinear polynomial rate	$\exp(w_1 \ln x + w_0)$	1	1	2	$0 < w_1 < 1$
Logarithmic rate	$w_1 \ln x + w_0$	1	1	2	$w_1 > 0$
Slow convergence	$w_0 + w_1/x$	1	1	2	$w_1 \neq 0$
Fast convergence	$w_0 + w_1 \cdot \exp(-x)$	1	1	2	$w_1 \neq 0$
Other					
Soft ReLu	$\ln(1 + e^x)$	1	1	0	
Sigmoid	$1/(w_0 + \exp(-w_1x))$	1	1	2	$w_1 > 0$
Nonparametric log-sigmoid	$1/(1 + \exp(-x))$	1	1	0	
Hiberbolic tangent	$\tanh(x)$	1	1	0	
softsign	$\frac{ x }{1+ x }$	1	1	0	

obtain the maximum likelihood estimate

$$\hat{y} = \hat{\mathbf{w}}^\top \mathbf{x}, \quad \hat{\mathbf{w}} = \arg \max_{\mathbf{w}} \frac{1}{2\beta} \sum_{i=1}^m (y_i - \mathbf{w}^\top \mathbf{x}_i)^2$$

for the output.

Table 5: Multivariate.

Bivariate				
Plus	$x_1 + x_2$	1	2	0
Minus	$x_1 - x_2$	1	2	0
Product	$x_1 \cdot x_2$	1	2	0
Division	$\frac{x_1}{x_2}$	1	2	0
	$x_1 \sqrt{x_2}$	1	2	0
	$x_1 \ln x_2$	1	2	0
Multivariate				
Sum of products	$\sum_{i,j} x_i x_j$	1	$n \geq 2$	0
Sum of products	$\sum_{i,j,k} x_i x_j x_k$	1	$n \geq 3$	0
Sum of Gaussians	$\sum_{j=1}^n a_j \exp(-\frac{(x_j - b_j)^2}{c_j})$	1	n	$3n$
Polynomial	$\sum_{j=0}^n a_j x^j$	1	1	n
Rational polynomial	$\frac{\sum_{j=0}^n a_j x^j}{x^m + \sum_{j=0}^{m-1} b_j x^j}$	1	1	$n + m + 1$

Table 6: Data statistics.

sum	$\sum_i x_i$	1	m	0
mean	$(\sum_i x_i)/m$	1	m	0
min	$\min_i x_i$	1	m	0
max	$\max_i x_i$	1	m	0
std	$\frac{1}{m-1} \sqrt{\sum_i (x_i - \text{mean}(x))^2}$	1	m	0
hist	$\sum_i [X_{j-1} < x_i \leq X_j]$	n	m	$n - 1$
conv	$\sum_j x_{i-j} w_j$	1	$m - n + 1$	$n \leq m$
FFT coefficients		n	m	1

5.1 EM-algorithm for mixture models

Assume the target variable \mathbf{y} is generated by one of K linear models $f_k(\mathbf{x}, \mathbf{w}_k)$. Let the distribution of the target variable \mathbf{y} be a mixture of normal distributions

$$p(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{y}|\mathbf{w}_k^\top \mathbf{x}, \beta) = \sum_{k=1}^K \frac{1}{(2\pi\beta_k)^{n/2}} \exp\left(-\frac{1}{2\beta_k}(\mathbf{y} - \mathbf{w}_k^\top \mathbf{x})^\top (\mathbf{y} - \mathbf{w}_k^\top \mathbf{x})\right). \quad (6)$$

Here $\boldsymbol{\theta}$ denotes the concatenated vector of parameters:

$$\boldsymbol{\theta} = [\mathbf{w}_1, \dots, \mathbf{w}_k, \boldsymbol{\pi}, \beta]^\top,$$

where $\boldsymbol{\pi} = [\pi_1, \dots, \pi_k]$ are weights of the models, and $\mathbf{B} = \beta \mathbf{I}_m$ is the covariance matrix for \mathbf{y} .

Parameter estimation. The goal is to find parameters vector $\hat{\boldsymbol{\theta}}$ which optimizes log-likelihood function for given data set D

$$\hat{\boldsymbol{\theta}} = \arg \max_{\boldsymbol{\theta}} \ln p(\mathbf{y}|\boldsymbol{\theta}), \quad \ln p(\mathbf{y}|\boldsymbol{\theta}) = \sum_{i=1}^m \ln \left(\sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{y}|\mathbf{w}_k^\top \mathbf{x}_i, \beta) \right). \quad (7)$$

To obtain maximum likelihood estimates (7) for parameter $\boldsymbol{\theta}$ of the model (6), let us introduce hidden indicator variables

$$Z = [\mathbf{z}_1, \dots, \mathbf{z}_m], \quad z_{ik} \in \{0, 1\},$$

such that

$$z_{ik} = 1 \Leftrightarrow y_i \sim \mathcal{N}(\mathbf{w}_k^\top \mathbf{x}_i, \beta).$$

Then the loglikelihood function $p(\mathbf{y}, Z|X, \boldsymbol{\theta})$ takes the form

$$\begin{aligned} p(\mathbf{y}|X, Z, \boldsymbol{\theta}) &= \sum_{i=1}^m \sum_{k=1}^K z_{ik} (\ln \pi_k + \ln \mathcal{N}(y_i|\mathbf{w}_k^\top \mathbf{x}_i, \beta)) = \\ &= \sum_{i=1}^m \sum_{k=1}^K z_{ik} \left(\ln \pi_k - \frac{1}{2\beta} (y_i - \mathbf{w}_k^\top \mathbf{x}_i)^2 + \frac{n \ln \beta}{2} + \text{const} \right). \end{aligned}$$

Since $p(\mathbf{y}, Z|X, \boldsymbol{\theta})$ depends on random variables z_{ik} , instead of $p(\mathbf{y}|X, \boldsymbol{\theta})$ maximize the expected loglikelihood of the observed data D :

$$\mathbb{E}_Z[p(\mathbf{y}, Z|X, \boldsymbol{\theta})] = \sum_{i=1}^m \sum_{k=1}^K \gamma_{ik} \left(\ln \pi_k - \frac{1}{2\beta} (y_i - \mathbf{w}_k^\top \mathbf{x}_i)^2 + \frac{n \ln \beta}{2} \right), \quad \gamma_{ik} = \mathbb{E}[z_{ik}|\mathbf{y}, X].$$

Finally, apply Expectation-Maximization algorithm to maximize $\mathbb{E}_Z[p(\mathbf{y}, Z|X, \boldsymbol{\theta})]$ updating parameters estimates $\boldsymbol{\theta}^{(r)}$ in two iterative steps.

E-step: obtain $\mathbb{E}(Z)$. Let $\Gamma = [\gamma_{ik}]$ be a matrix of posterior probabilities that i -th sample is generated by k -th model. Using Bayesian rule, obtain

$$\gamma_{ik}^{(r+1)} = \mathbb{E}(z_{ik}) = p(k|\mathbf{x}_i, \boldsymbol{\theta}^{(r)}) = \frac{\pi_k \mathcal{N}(y_i|\mathbf{x}_i^\top \mathbf{w}_k^{(r)}, \beta^{(r)})}{\sum_{k'=1}^K \pi_{k'} \mathcal{N}(y_i|\mathbf{x}_i^\top \mathbf{w}_{k'}^{(r)}, \beta^{(r)})}. \quad (8)$$

Define expectations of joint loglikelihood $\ln p(\mathbf{y}, Z|X, \boldsymbol{\theta})$ with respect to the posteriors distribution $p(Z|\mathbf{y}, \boldsymbol{\theta})$

$$Q^{(r)}(\boldsymbol{\theta}) = \mathbb{E}_Z(\ln p(\mathbf{y}, Z|\boldsymbol{\theta})) = \sum_{i=1}^m \sum_{k=1}^K \gamma_{ik}^{(r+1)} \left(\ln \pi_k^{(r)} + \ln \mathcal{N}(y_i | \mathbf{x}_i^\top \mathbf{w}_k^{(r)}, \beta^{(r)}) \right). \quad (9)$$

M-step: update parameters $\boldsymbol{\theta}$, maximizing $Q^{(r)}(\boldsymbol{\theta})$. Maximize function $Q^{(r)}(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$ with $\Gamma^{(r+1)}$ fixed. First, optimize π_k , which is constrained as $\sum_{k=1}^K \pi_k = 1$. Using Lagrange multipliers, obtain the following estimation

$$\pi_k^{(r+1)} = \frac{1}{n} \sum_{i=1}^m \gamma_{ik}^{(r+1)}.$$

Next, maximize $Q^{(r)}$ with respect to \mathbf{w}_k for k -th model. With π_k fixed maximizing (9) is equivalent to

$$\begin{aligned} \mathbf{w}_k^{(r+1)} &= \arg \max_{\mathbf{w}_k} \sum_{i=1}^m -\gamma_{ik}^{(r+1)} (y_i - \mathbf{w}_k^\top \mathbf{x}_i)^2, \\ \beta_k^{(r)} &= \arg \max_{\beta} \sum_{i=1}^m \gamma_{ik}^{(r+1)} \left(n \ln \beta - \frac{1}{\beta} (y_i - \mathbf{x}_i^\top \mathbf{w}_k^{(r+1)})^2 \right). \end{aligned}$$

5.2 Mixture of experts

Suppose that each model $f(\mathbf{x}, \mathbf{w}_k)$ generates a sample (\mathbf{x}, y) with some probability $p(k|\mathbf{x}, \mathbf{w})$. Then the following factorization holds

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \sum_{k=1}^K p(y, k|\mathbf{x}, \boldsymbol{\theta}) = \sum_{k=1}^K p(k|\mathbf{x}, \boldsymbol{\theta}) p(y|k, \mathbf{x}, \boldsymbol{\theta})$$

for $p(y|\mathbf{x}, \boldsymbol{\theta})$. Here $p(k|\mathbf{x}, \boldsymbol{\theta})$ correspond to weight parameters π_k in (6) dependent on the inputs \mathbf{x} . Assuming normal linear models $f(\mathbf{x}, \mathbf{w}_k)$ or, equivalently, normal distributions $p(y|\mathbf{x}, \mathbf{w}_k) = \mathcal{N}(y|\mathbf{w}_k^\top \mathbf{x}, \beta)$, obtain

$$p(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k(\mathbf{x}, \mathbf{v}_k) \mathcal{N}(\mathbf{y} | \mathbf{w}_k^\top \mathbf{x}, \beta), \quad (10)$$

where

$$\pi_k(\mathbf{x}, \mathbf{v}_k) = \frac{\exp(\mathbf{v}_k^\top \mathbf{x})}{\sum_{k'=1}^K \exp(\mathbf{v}_{k'}^\top \mathbf{x})}.$$

The difference between mixture of experts model (10) and mixture model (6) is that model weights π_k depend on inputs \mathbf{x} in mixture of experts. Similarly, EM-procedure for mixture of experts differs from EM-procedure for mixture models in the way γ_{ik} are optimized in M-step.

Algorithm 3: EM-algorithm for mixture of experts.

begin

Data: (\mathbf{x}_i, y_i) , $i = 1, \dots, m$. Parameters: number of experts K .

Result: Parameters $\boldsymbol{\theta}$ of the model (10).

Initialize $[\mathbf{w}, \beta, \mathbf{v}] \equiv \boldsymbol{\theta} = \boldsymbol{\theta}^{(0)}$, $r = 0$

while $\boldsymbol{\theta}$ keeps changing **do**

E step: compute hidden variables $\gamma_{ik}^{(r+1)}$, the expectation of the indicator variables, using (8)

M step: find new parameter estimates

$$\mathbf{v}_k^{(r+1)} = \arg \max_{\mathbf{v}} Q_k^{(r), \mathbf{v}}(\mathbf{v}), \quad Q_k^{(r), \mathbf{v}}(\mathbf{v}) = \sum_{i=1}^m \gamma_{ik}^{(r+1)} \ln \pi_k(\mathbf{x}_i, \mathbf{v})$$

$$\mathbf{w}_k^{(r+1)} = \arg \max_{\mathbf{w}_k} Q_k^{(r), \mathbf{w}}(\mathbf{w}_k), \quad Q_k^{(r), \mathbf{w}}(\mathbf{w}_k) = \sum_{i=1}^m \gamma_{ik}^{(r+1)} (y_i - \mathbf{w}_k^\top \mathbf{x}_i)^2,$$

$$\beta_k^{(r+1)} = \arg \max_{\beta} Q_k^{(r), \beta}(\beta), \quad Q_k^{(r), \beta}(\beta) = \left(n \ln \beta - \frac{1}{\beta} (y_i - \mathbf{x}_i^\top \mathbf{w}_k^{(r+1)})^2 \right)$$

5.3 Distance between two models of N time series

Introduce a distance function $\rho(f_k, f_l)$ between two models. Use the Jensen-Shannon divergence; $\rho_{kl} \in [0, 1]$ is a metric:

$$\rho(p_k \| p_l) = 2^{-1} D_{\text{KL}}(p_k \| p') + 2^{-1} D_{\text{KL}}(p' \| p_l),$$

where $p' = 2^{-1}(p_k + p_l)$ and $p_k \stackrel{\text{def}}{=} (p(\mathbf{w}|D, A, B, f_k))$. The non-symmetric Kullback-Leibler divergence is

$$D_{\text{KL}}(p \| p') = \int_{\mathbf{w} \in \mathbb{W}} p'(\mathbf{w}) \ln \frac{p(\mathbf{w})}{p'(\mathbf{w})} d\mathbf{w}.$$

6 Computational experiment

The goal of the experiment is to compare the following four approaches to the multiscale forecasting: 1) Bayesian mixture model approach, 2) random multumodel, 3) vector random decision forest and 4) vector adaboost. The last two algorithms are modifications of

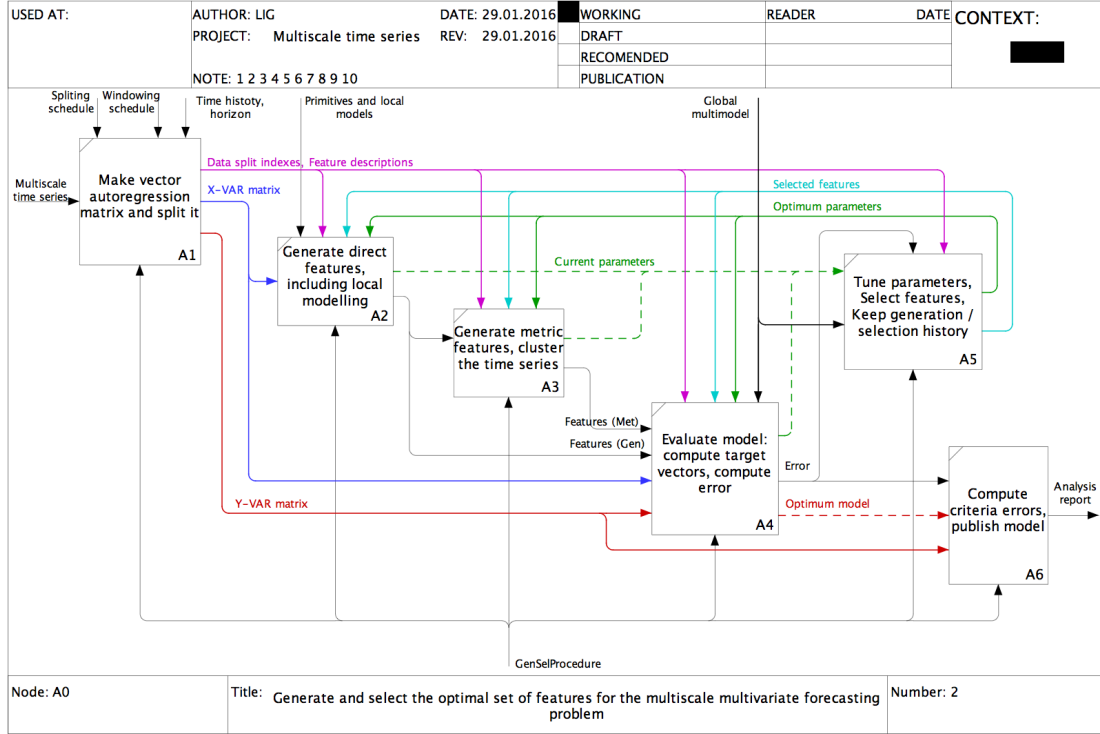


Figure 5: Multiscale forecasting pipeline.

[link]. The modifications are needed to produce the vector of multiscale time series as their outputs. The experiment is performed on 1) non-modified autoregression data and on 2) data with additionally generated features as it is described in the corresponding section.

7 Appendix: Discrete genetic algorithm for feature selection (will be converted to bootstrap random linear multimodel algorithm)

1. There are set of binary vectors $\{\mathbf{a}_1, \dots, \mathbf{a}_P\}$, $\mathbf{a} \in \{0, 1\}^n$;
2. get two vectors $\mathbf{a}_p, \mathbf{a}_q$, $p, q \in \{1, \dots, P\}$;
3. chose random number $\nu \in \{1, \dots, n - 1\}$;
4. split both vectors and change their parts:

$$[a_{p,1}, \dots, a_{p,\nu}, a_{q,\nu+1}, \dots, a_{q,n}] \rightarrow \mathbf{a}'_p,$$

$$[a_{q,1}, \dots, a_{q,\nu}, a_{p,\nu+1}, \dots, a_{p,n}] \rightarrow \mathbf{a}'_q;$$

5. choose random numbers $\eta_1, \dots, \eta_Q \in \{1, \dots, n\}$;
6. invert positions η_1, \dots, η_Q of the vectors $\mathbf{a}'_p, \mathbf{a}'_q$;
7. repeat items 2-6 $P/2$ times;
8. evaluate the obtained models.

Repeat R times; here P, Q, R are the parameters of the algorithm and n is the number of the corresponding model features.

8 Appendix: Mixture modelling under random bootstrapped models

Denote the indexes of objects as $\{1, \dots, i, \dots, m\} = \mathcal{I}$, the split $\mathcal{I} = \mathcal{B}_1 \sqcup \dots \sqcup \mathcal{B}_K$ and the indexes of features as $\{1, \dots, j, \dots, n\} = \mathcal{J}$, the active set $\mathcal{A}_k \subseteq \mathcal{J}$.

Let the regression model

$$\mathbf{f} : (\mathbf{w}, \mathbf{x}) \mapsto \mathbf{y};$$

with the selected model of optimal structure

$$\mathbf{E}(\mathbf{y}_i | \mathbf{x}) = \mathbf{W}_{\mathcal{A}} \mathbf{x}_i.$$

The multimodel \mathbf{f} is a set of the models $\mathbf{f} = \{\mathbf{f}_k \mid k = 1, \dots, K\}$, such that for each k

$$\mathbf{E}(y_{i \in \mathcal{B}_k} | \mathbf{x}) = \mathbf{W}_{\mathcal{A}_k} \mathbf{x}_{i \in \mathcal{B}_k} \quad \text{with} \quad \mathcal{I} = \sqcup_{k=1}^K \mathcal{B}_k \ni i.$$

State the multimodel selection problem as follows. An optimal single model is

$$\hat{\mathbf{f}}(\mathbf{w}, \mathbf{x}) = \arg \max_{\mathcal{A} \subseteq \mathcal{J}} \mathcal{E}(\mathbf{f}(\mathbf{w}_{\mathcal{A}}, \mathbf{x})),$$

where \mathcal{E} denotes the model evidence in coherent Bayesian inference. An optimal multilevel model is

$$\hat{\mathbf{f}}(\mathbf{w}_1, \dots, \mathbf{w}_K, \mathbf{x}) = \arg \max_{\sqcup_{k=1}^K \mathcal{B}_k = \mathcal{I}} \prod_{k=1}^K \mathcal{E}(\mathbf{f}(\mathbf{w}_k, \mathbf{x}_{\mathcal{B}_k})).$$

The model difference must be statistically significant

$$\mathcal{F} \supset \hat{\mathbf{f}} = \arg \max_{\mathcal{B}_1, \mathcal{B}_2 \subset \mathcal{B}} \rho(f_1, f_2)$$

given set of indices $\hat{\mathcal{A}}$, such that

$$\hat{\mathcal{A}} = \arg \max_{\mathcal{A} \subseteq \mathcal{I}} \mathcal{E}(\mathbf{f}_1(\mathbf{w}_{\mathcal{A}}, \mathbf{x}^{\mathcal{B}_1})) \mathcal{E}(\mathbf{f}_2(\mathbf{w}'_{\mathcal{A}}, \mathbf{x}^{\mathcal{B}_2})) .$$

References

- [1] Rob J. Hyndman. Another look at forecast-accuracy metrics for intermittent demand. *Foresight*, (4):43–46, June 2006.