

Feature generation for multiscale time series forecasting

A. Motrenko, R. Neychev, R. Isachenko, M. Popova, V. Strijov

Moscow Institute of Physics and Technology

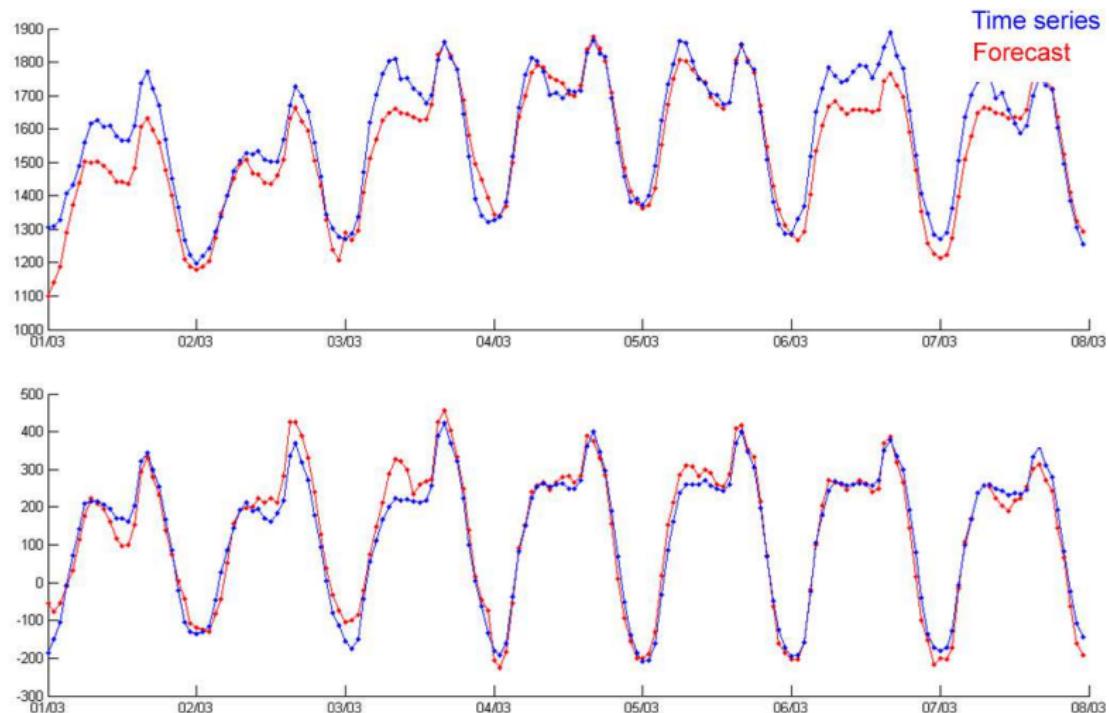
2016

Outline

- ▶ Design matrix
- ▶ Testing procedure
- ▶ Feature generation
- ▶ Feature selection
- ▶ Mixture models
- ▶ Resampling

Problem statement

Energy consumption one-week forecast for each hour



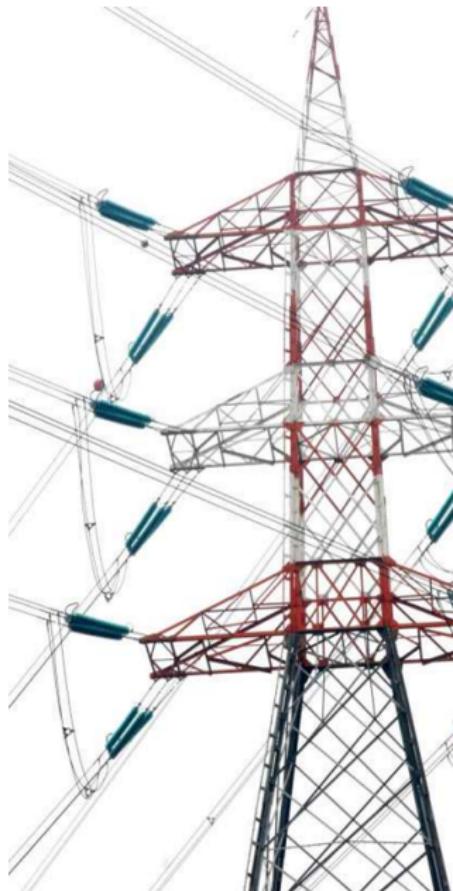
The periodic components of the multivariate time series

The time series:

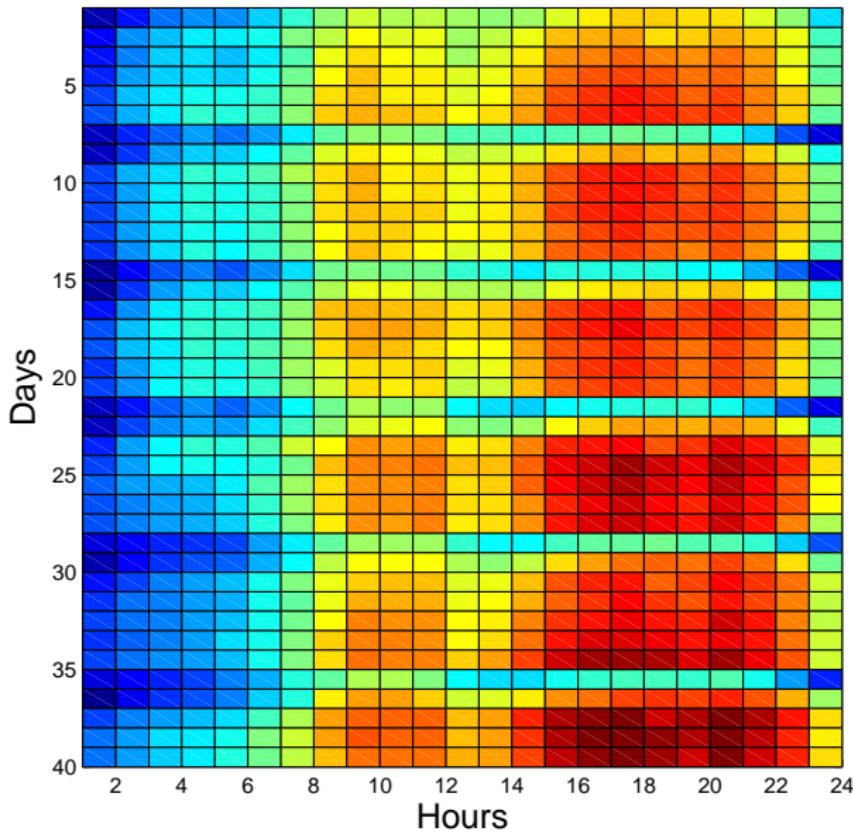
- ▶ energy price,
- ▶ consumption,
- ▶ daytime,
- ▶ temperature,
- ▶ humidity,
- ▶ wind force,
- ▶ holiday schedule.

Periods:

- ▶ one year seasons (temperature, daytime),
- ▶ one week,
- ▶ one day (working day, week-end),
- ▶ a holiday,
- ▶ aperiodic events.



The autoregressive matrix, five week-ends



The autoregressive matrix and the linear model

$$\mathbf{X}^*_{(m+1) \times (n+1)} = \left(\begin{array}{c|cccc} s_T & s_{T-1} & \dots & s_{T-\kappa+1} \\ \hline s_{(m-1)\kappa} & s_{(m-1)\kappa-1} & \dots & s_{(m-2)\kappa+1} \\ \dots & \dots & \dots & \dots \\ s_{n\kappa} & s_{n\kappa-1} & \dots & s_{n(\kappa-1)+1} \\ \dots & \dots & \dots & \dots \\ s_\kappa & s_{\kappa-1} & \dots & s_1 \end{array} \right).$$

In a nutshell,

$$\mathbf{X}^* = \left[\begin{array}{c|c} s_T & \mathbf{x}_{m+1} \\ \hline 1 \times 1 & 1 \times n \\ \mathbf{y} & \mathbf{X} \\ m \times 1 & m \times n \end{array} \right].$$

In terms of linear regression:

$$\mathbf{y} = \mathbf{X}\mathbf{w},$$

$$y_{m+1} = s_T = \mathbf{w}^T \mathbf{x}_{m+1}^T.$$

Model generation

Introduce a set of the primitive functions $\mathfrak{G} = \{g_1, \dots, g_r\}$,
for example $g_1 = 1$, $g_2 = \sqrt{x}$, $g_3 = x$, $g_4 = x\sqrt{x}$, etc.

The generated set of features $\mathbf{X} =$

$$\left(\begin{array}{ccc|c|ccc} g_1 \circ s_{T-1} & \dots & g_r \circ s_{T-1} & \dots & g_1 \circ s_{T-\kappa+1} & \dots & g_r \circ s_{T-\kappa+1} \\ g_1 \circ s_{(m-1)\kappa-1} & \dots & g_r \circ s_{(m-1)\kappa-1} & \dots & g_1 \circ s_{(m-2)\kappa+1} & \dots & g_r \circ s_{(m-2)\kappa+1} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ g_1 \circ s_{n\kappa-1} & \dots & g_r \circ s_{n\kappa-1} & \dots & g_1 \circ s_{n(\kappa-1)+1} & \dots & g_r \circ s_{n(\kappa-1)+1} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ g_1 \circ s_{\kappa-1} & \dots & g_r \circ s_{\kappa-1} & \dots & g_1 \circ s_1 & \dots & g_r \circ s_1 \end{array} \right).$$

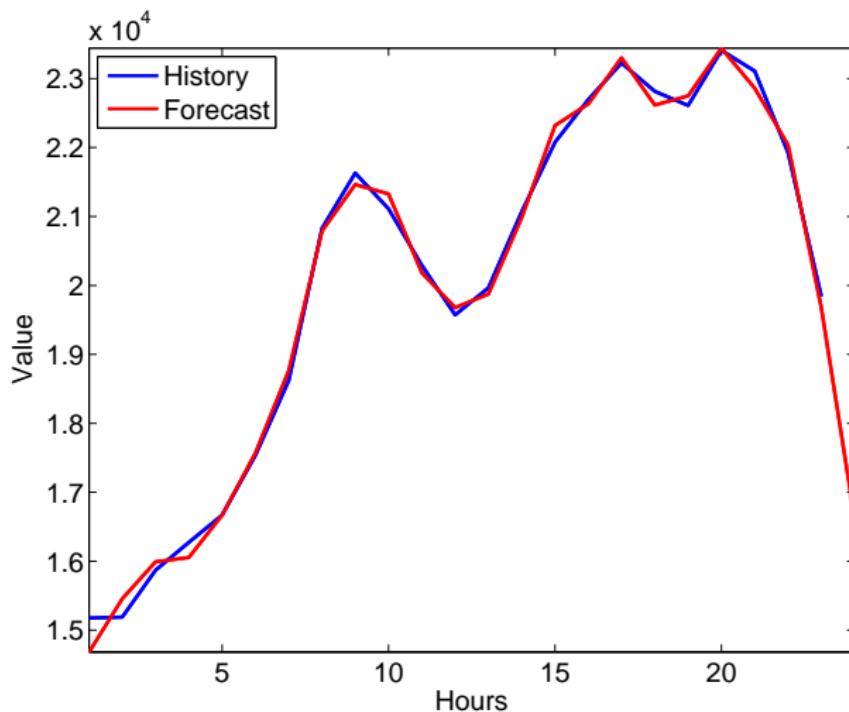
Kolmogorov-Gabor polynomial as a variant for model generation

$$y = w_0 + \sum_{i=1}^{UV} w_i x_i + \sum_{i=1}^n \sum_{j=1}^n w_{ij} x_i x_j + \dots + \sum_{i=1}^n \dots \sum_{z=1}^n w_{i\dots z} x_i \dots x_z,$$

where the coefficients

$$\mathbf{w} = (w_0, w_i, w_{ij}, \dots, w_{i\dots z})_{i,j,\dots,z=1,\dots,n}.$$

The one-day forecast (an example)



The function $y = f(\mathbf{x}, \mathbf{w})$ could be a linear model, neural network, deep NN, SVN, ...

III-conditioned matrix, or curse of dimensionality

Assume we have hourly data on price/consumption for three years.
Then the matrix \mathbf{X}^*
 $(m+1) \times (n+1)$ is

156×168 , in details: $52w \cdot 3y \times 24h \cdot 7d$;

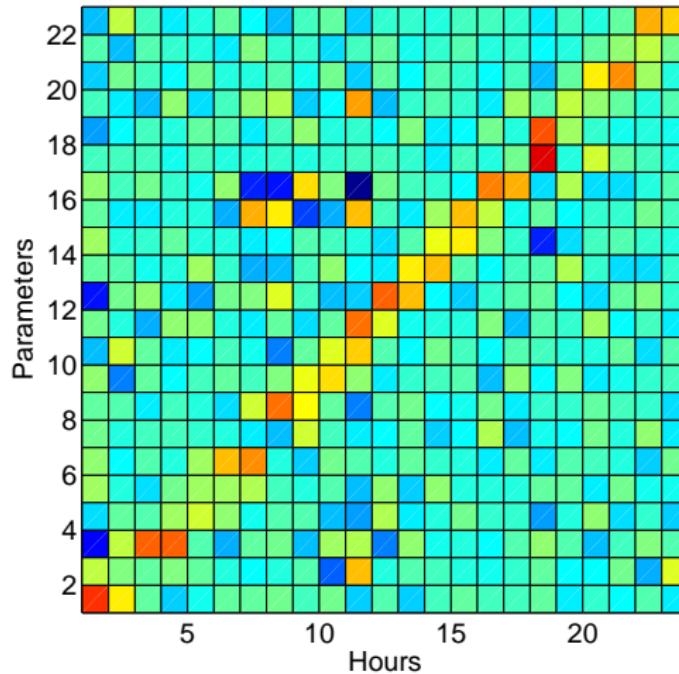
- ▶ for 6 time series the matrix \mathbf{X} is 156×1008 ,
- ▶ for 4 primitive functions it is 156×4032 ,

$$m \ll n.$$

The autoregressive matrix could be considered as *ill-conditioned* and *multi-correlated*. The model selection procedure is required.

How many parameters must be used to forecast?

The color shows the value of a parameter for each hour.



Estimate parameters $\mathbf{w}(\tau) = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$, then calculate the sample $s(\tau) = \mathbf{w}^T(\tau) \mathbf{x}_{m+1}$ for each τ of the next ($m+1$ -th) period.

Ways to model selection: brief list of algorithms

Exhaustive search and modifications

1. Exhaustive search of 2^P models
2. Genetic algorithms
3. Add/Del (append/delete a feature), $P(P - 1)/2$ models
4. Add-del or stepwise regression, $\sim P^2$ models

Parameter space analysis

1. Least angle regression, Lasso, Stagewise, Elastic net
2. Optimal brain damage/surgery

Exhaustive search and Add algorithms

The initial model includes all independent variables

$$f(\mathbf{w}, \mathbf{x}) = \alpha_1 w_1 x_1 + \alpha_2 w_2 x_2 + \dots + \alpha_n w_n x_n.$$

The hyperparameter $\alpha \in \{0, 1\}$ is included in the model. The **exhaustive search** procedure counts

α_1	α_2	\dots	α_n
1	0	\dots	0
0	1	\dots	0
\dots	\dots	\dots	\dots
1	1	\dots	1

Add (append a feature)

Step 0. The active set $\mathcal{A}_0 = \emptyset$.

Step $k = 1, \dots, n$. Select the next best feature index

$$\hat{j} = \arg \min_{j \in \{1, \dots, n\} \setminus \mathcal{A}_k} \min_{\mathbf{w} \in \mathbb{R}^{|\mathcal{A}|}} \|[\mathbf{X}_{\mathcal{A}_k} \boldsymbol{\chi}_j] \mathbf{w} - \mathbf{y}\|_2^2,$$

according to minimum of the error function $S(\mathbf{w})$; then

$$\mathcal{A}_{k+1} = \mathcal{A}_k \cup \hat{j}.$$

Discrete genetic algorithm for feature selection (simple ver.)

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:

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

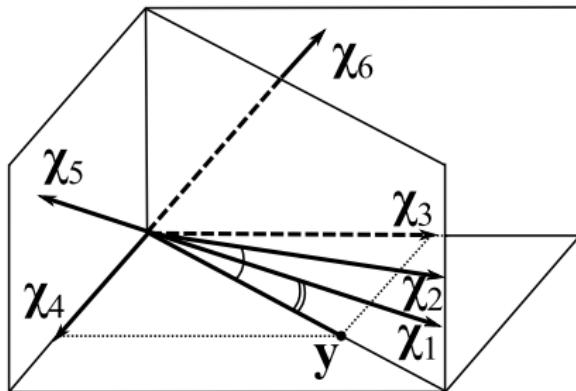
$$[a_{q,1}, \dots, a_{q,\nu}, a_{p,\nu+1}, \dots, a_{p,n}] \rightarrow \mathbf{a}'_q;$$

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.

Selection of a stable set of features of restricted size

The sample contains multicollinear χ_1, χ_2 and noisy χ_5, χ_6 features, columns of the design matrix \mathbf{X} . We want to select two features from six.



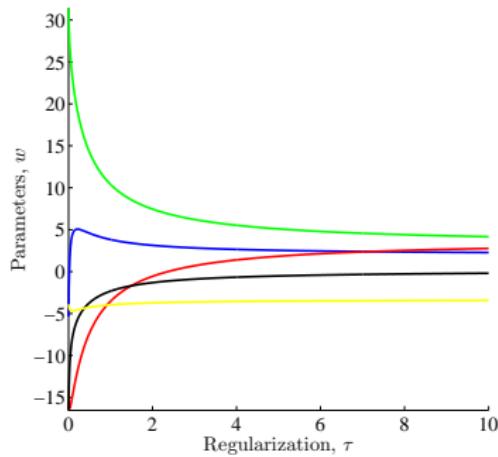
Stability and accuracy for a fixed complexity

The solution: χ_3, χ_4 is an orthogonal set of features minimizing the error function.

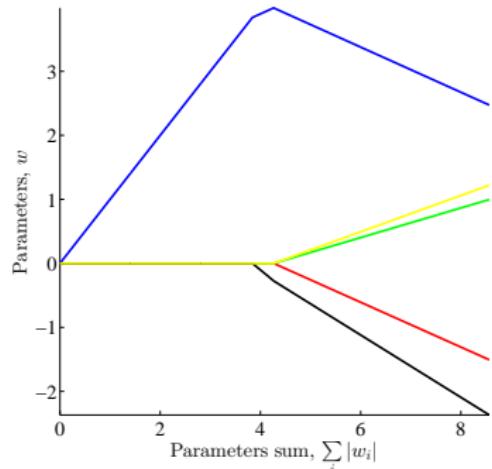
Algorithms: GMDH, Stepwise, Ridge, Lasso, Stagewise, FOS, LARS, Genetics, ...

Model parameter values with regularization

Vector-function $\mathbf{f} = \mathbf{f}(\mathbf{w}, \mathbf{X}) = [f(\mathbf{w}, \mathbf{x}_1), \dots, f(\mathbf{w}, \mathbf{x}_m)]^T \in \mathbb{Y}^m$.



$$S(\mathbf{w}) = \|\mathbf{f}(\mathbf{w}, \mathbf{X}) - \mathbf{y}\|^2 + \gamma^2 \|\mathbf{w}\|^2$$



$$S(\mathbf{w}) = \|\mathbf{f}(\mathbf{w}, \mathbf{X}) - \mathbf{y}\|^2, \\ T(\mathbf{w}) \leq \tau$$

Multiscale data

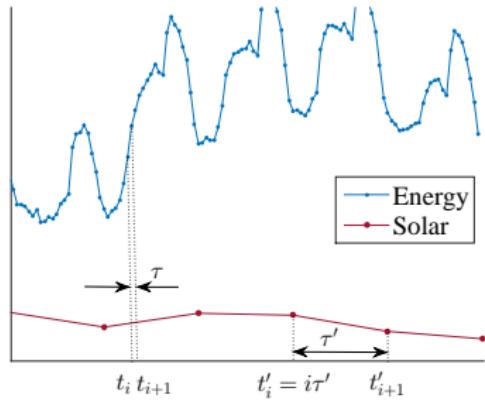
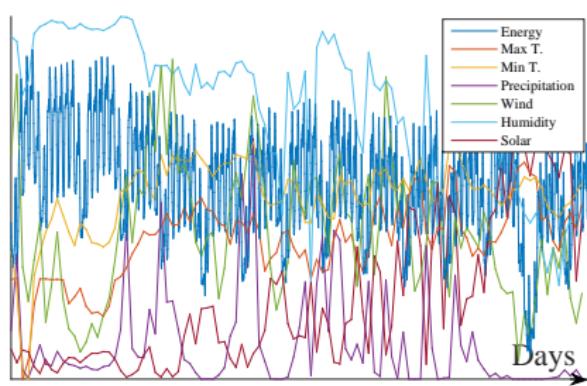
Consider a large set of time series $\mathfrak{D} = \{\mathbf{s}^{(q)} | q = 1 \dots, Q\}$.

Each real-valued time series \mathbf{s}

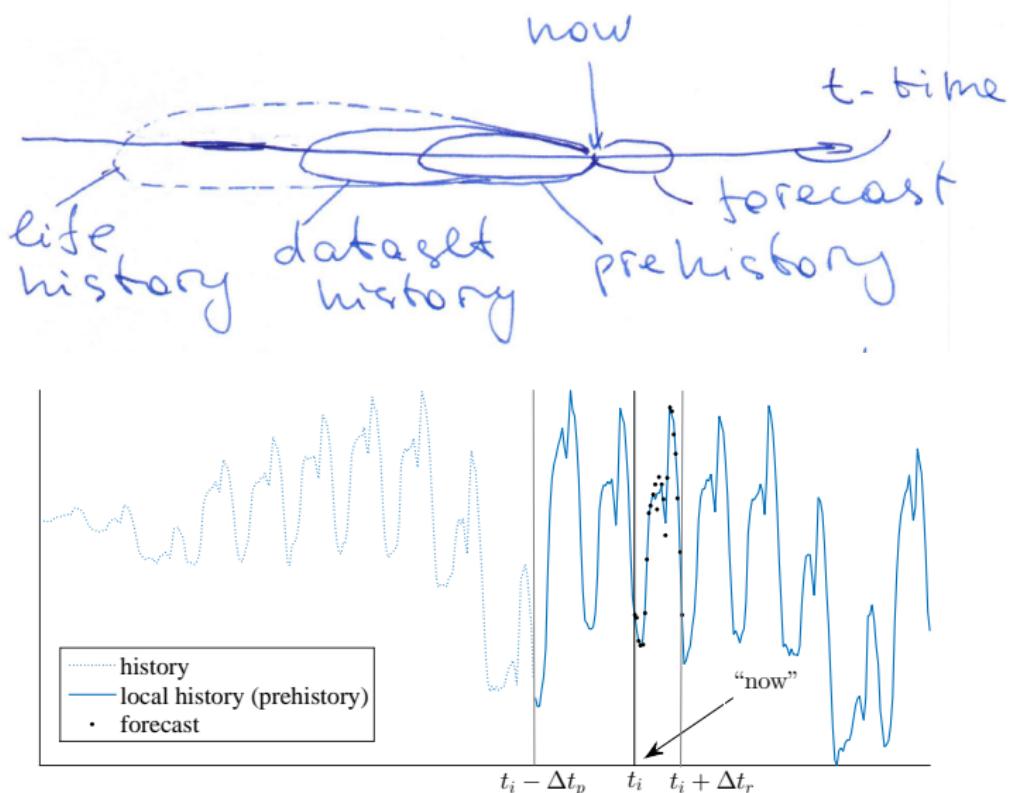
$$\mathbf{s} = [s_1, \dots, s_i, \dots, s_T], \quad s_i = s(t_i), \quad 0 \leq t_i \leq t_{\max}$$

is a sequence of observations of some real-valued signal $s(t)$.

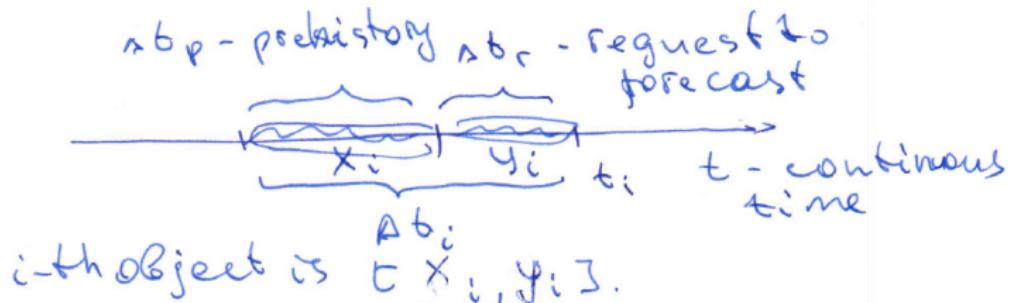
Each time series $\mathbf{s}^{(q)}$ has its own sampling rate $\tau^{(q)}$.



Time series forecasting

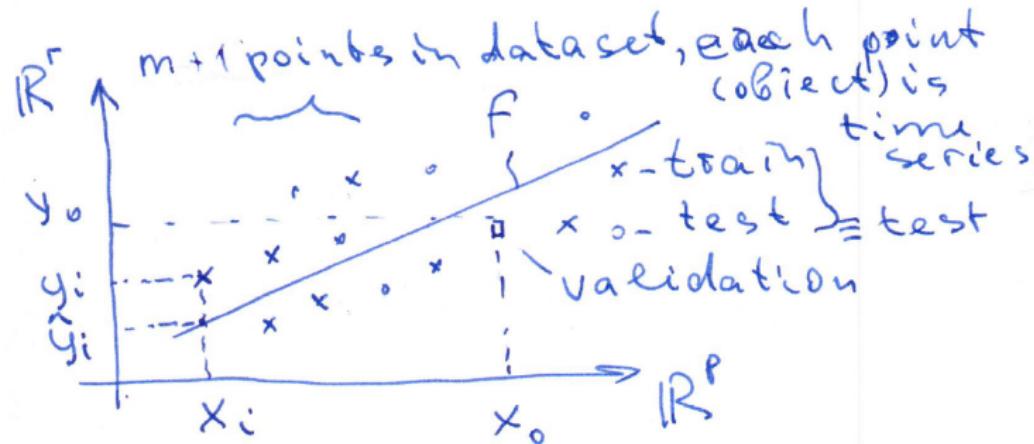


Design matrix



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

Design matrix



$$\mathbf{X}^* = \left[\begin{array}{c|c} \mathbf{x} & \mathbf{y} \\ \hline 1 \times n & 1 \times r \\ \mathbf{X} & \mathbf{Y} \\ m \times n & m \times r \end{array} \right] = \left[\begin{array}{ccc|ccc} \mathbf{x}^{(1)} & \dots & \mathbf{x}^{(Q)} & \mathbf{y}^{(1)} & \dots & \mathbf{y}^{(Q)} \\ \hline \mathbf{x}_m^{(1)} & \dots & \mathbf{x}_m^{(Q)} & \mathbf{y}_m^{(1)} & \dots & \mathbf{y}_m^{(Q)} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_1^{(1)} & \dots & \mathbf{x}_1^{(Q)} & \mathbf{y}_1^{(1)} & \dots & \mathbf{y}_1^{(Q)} \end{array} \right].$$

Regression problem

Now we are able to state the regression problem as follows:

$$\hat{\mathbf{y}} = f(\mathbf{x}, \hat{\mathbf{w}}), \quad \hat{\mathbf{w}} = \arg \min_{\hat{\mathbf{w}}} S(\mathbf{w} | \mathbf{f}(\mathbf{w}, \mathbf{x}), \mathbf{y}). \quad (1)$$

Here the error function $S(\mathbf{w} | \mathbf{f}(\mathbf{w}, \mathbf{x}), \mathbf{y})$ averages forecasting errors of $[\mathbf{x}_i | \mathbf{y}_i]$ over all segments $i = 1, \dots, m$ in the test set:

$$S(\mathbf{w} | \mathbf{f}(\mathbf{w}, \mathbf{x}), \mathbf{y}) = \frac{r}{m} \sum_{i=1}^m I(\mathbf{y}_i, f(\mathbf{x}_i, \mathbf{w})).$$

Let $\boldsymbol{\varepsilon}$ denote residual vector

$$\boldsymbol{\varepsilon} = [\varepsilon_1, \dots, \varepsilon_r] = \mathbf{y} - \hat{\mathbf{y}}$$

for the forecast $\hat{\mathbf{y}} = \mathbf{f}(\mathbf{w}, \mathbf{x})$ of \mathbf{y} .

Types of forecasting errors

- ▶ scale-dependent metrics: mean absolute error

$$MAE = \frac{1}{r} \sum_{j=1}^r |\varepsilon_j|,$$

- ▶ percentage-error metrics: (symmetric) mean absolute percent error

$$MAPE = \frac{1}{r} \sum_{j=1}^r \frac{|\varepsilon_j|}{|y_j|}, \quad sMAPE = \frac{1}{r} \sum_{j=1}^r \frac{2|\varepsilon_j|}{|\hat{y}_j + y_j|},$$

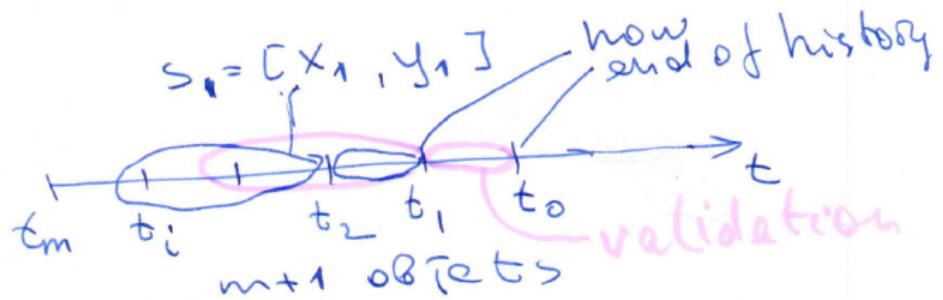
- ▶ relative-error metrics (to residues ε^* of a benchmark method):

$$MRAE = \frac{1}{r} \sum_{j=1}^r \frac{|\varepsilon_j|}{\varepsilon_j^*},$$

- ▶ and scale-free error metrics:

$$MASE = \frac{n-1}{r} \frac{\sum_{i=1}^r |\varepsilon_j|}{\sum_{j=2}^n |x_j - x_{j-1}|}.$$

Rolling validation



Rolling validation

- 1) construct the validation vector $\mathbf{x}_{\text{val},k}^*$ for time series of the length Δt_r as the first row of the design matrix \mathbf{Z} ,
- 2) construct the rest rows of the design matrix \mathbf{Z} for the time after t_k and present it as

$$\mathbf{Z} = \left[\begin{array}{c|c} \dots & \dots \\ \hline \mathbf{x}_{\text{val},k} & \mathbf{y}_{\text{val},k} \\ 1 \times n & 1 \times r \\ \hline \mathbf{X}_{\text{train},k} & \mathbf{Y}_{\text{train},k} \\ m_{\min} \times n & m_{\min} \times r \\ \hline \dots & \dots \end{array} \right], \quad \uparrow k$$

- 3) optimize model parameters \mathbf{w} using $\mathbf{X}_{\text{train},k}$, $\mathbf{Y}_{\text{train},k}$,
- 4) compute residues $\varepsilon_k = \mathbf{y}_{\text{val},k} - \mathbf{f}(\mathbf{x}_{\text{val},k}, \mathbf{w})$ and MAPE,
- 5) increment k and repeat.

Feature generation

Generating extra features

To augment feature description, consider the following types of features:

- 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.

Functional transforms

The procedure of generating new features ϕ requires:

- ▶ the original features $\mathbf{x} = \{\mathbf{x}_1, \dots, \mathbf{x}_Q\}$,
- ▶ the set of primitive functions $G = \{g(\mathbf{b}, \mathbf{x})\}$,

$$g : \mathbf{x} \mapsto \phi;$$

- ▶ the generation rules: $\mathcal{G} \supset G$, where the superposition $g_k \circ g_l \in \mathcal{G}$ w.r.t. numbers and types of the input and output arguments;
- ▶ the simplification rules: g_u is not in \mathcal{G} , if there exist a rule

$$r : g_u \mapsto g_v \in \mathcal{G}.$$

The result is

the set of the features $\mathbf{x} = \{\mathbf{x}_1, \dots, \mathbf{x}_Q, \phi_1, \dots, \phi_N\}$.

Examples of nonparametric transformation functions

► Univariate

Formula	Output dimension
\sqrt{x}	1
$x\sqrt{x}$	1
$\arctan x$	1
$\ln x$	1
$x \ln x$	1

► Bivariate

Plus	$x_1 + x_2$
Minus	$x_1 - x_2$
Product	$x_1 \cdot x_2$
Division	$\frac{x_1}{x_2}$
	$x_1 \sqrt{x_2}$
	$x_1 \ln x_2$

Nonparametric transformations: sample statistics

Nonparametric transformations include basic data statistics:

- ▶ Sum or average value of each row \mathbf{x}_i , $i = 1, \dots, m$:

$$\phi_i = \sum_{j=1}^n x_{ij}, \text{ or } \phi'_i = \frac{1}{n} \sum_{j=1}^n x_{ij}.$$

- ▶ Min and max values: $\phi_i = \min_j x_{ij}$, $\phi'_i = \max_j x_{ij}$.
- ▶ Standard deviation:

$$\phi_i = \frac{1}{n-1} \sqrt{\sum_{j=1}^n (x_{ij} - \text{mean}(\mathbf{x}_i))^2}.$$

- ▶ Data quantiles: $\phi_i = [X_1, \dots, X_K]$, where

$$\sum_{j=1}^n [X_{k-1} < x_{ij} \leq X_k] = \frac{1}{K}, \text{ for } k = 1, \dots, K.$$

Nonparametric transformations: Haar's transform

Applying Haar's transform produces multiscale representations of the same data.

Assume that $n = 2^K$ and init $\phi_{i,j}^{(0)} = \phi'_{i,j}^{(0)} = x_{ij}$ for $j = 1, \dots, n$.

To obtain coarse-graining and fine-graining of the input feature vector \mathbf{x}_i , for $k = 1, \dots, K$ repeat:

- ▶ data averaging step

$$\phi_{i,j}^{(k)} = \frac{\phi_{i,2j-1}^{(k-1)} + \phi_{i,2j}^{(k-1)}}{2}, \quad j = 1, \dots, \frac{n}{2^k},$$

- ▶ and data differencing step

$$\phi'_{i,j}^{(k)} = \frac{\phi'_{i,2j}^{(k-1)} - \phi'_{i,2j-1}^{(k-1)}}{2}, \quad j = 1, \dots, \frac{n}{2^k}.$$

The resulting multiscale feature vectors are $\phi_i = [\phi_i^{(1)}, \dots, \phi_i^{(K)}]$ and $\phi'_i = [\phi'_i^{(1)}, \dots, \phi'_i^{(K)}]$.

Parametric transformations

Optimization of the transformation function parameters \mathbf{b} is iterative:

1. Fix the vector $\hat{\mathbf{b}}$, collected over all the primitive functions $\{g\}$, which generate features ϕ :

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

2. Optimize transformation parameters $\hat{\mathbf{b}}$ given model parameters $\hat{\mathbf{w}}$

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

Repeat these steps until vectors $\hat{\mathbf{w}}, \hat{\mathbf{b}}$ converge.

Examples of parametric transformation functions

Function name	Formula	Output dim.	Num. of args	Num. of pars
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	$w_1 w_2 x^{w_2-1} \exp -w_1 x^{w_2}$	1	1	2
Weibull-3	$w_1 w_2 x^{w_2-1} \exp -w_1(x - w_3)^{w_2}$	1	1	3
...

Monotone functions

► By grow rate

Function name	Formula	Constraints
Linear	$w_1x + w_0$	
Exponential rate	$\exp(w_1x + w_0)$	$w_1 > 0$
Polynomial rate	$\exp(w_1 \ln x + w_0)$	$w_1 > 1$
Sublinear polynomial rate	$\exp(w_1 \ln x + w_0)$	$0 < w_1 < 1$
Logarithmic rate	$w_1 \ln x + w_0$	$w_1 > 0$
Slow convergence	$w_0 + w_1/x$	$w_1 \neq 0$
Fast convergence	$w_0 + w_1 \cdot \exp(-x)$	$w_1 \neq 0$

► Other

Soft ReLu	$\ln(1 + e^x)$	
Sigmoid	$1/(w_0 + \exp(-w_1x))$	$w_1 > 0$
Softmax	$1/(1 + \exp(-x))$	
Hiperbolic tangent	$\tanh(x)$	
softsign	$\frac{ x }{1+ x }$	

Parameters of the local models

Other options:

- ▶ Parameters of SSA approximation of the time series $\mathbf{x}^{(q)}$.
- ▶ Parameters of the FFT of each $\mathbf{x}^{(q)}$.
- ▶ Parameters of polynomial/spline approximation of each $\mathbf{x}^{(q)}$.

Parameters of the local models: SSA

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

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

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

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

For the original feature vector $\mathbf{x} = [\mathbf{x}^{(1)}, \mathbf{x}^{(Q)}]$ use the parameters $\phi(\mathbf{x}^{(q)})$, $q = 1, \dots, Q$ as the features.

Metric features: distances to the centroids of local clusters

Apply kernel trick to the time series.

1. For given local feature vector $\mathbf{x}_i^{(q)}$, $q = 1, \dots, Q$ compute k -means centroids $\mathbf{c}_p^{(m)}$, $p = 1, \dots, P$.
2. With the selected k -means distance function ρ construct the feature vector

$$\phi_i^{(q)} = [\rho(\mathbf{c}_1^{(q)}, \mathbf{x}_i^{(q)}), \dots, \rho(\mathbf{c}_P^{(q)}, \mathbf{x}_i^{(q)})] \in \mathbb{R}_+^P.$$

The procedure may be applied to each $\mathbf{x}^{(q)}$ or directly to the $\mathbf{x} = [\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(Q)}]$, resulting in only P additional features instead of $Q \cdot P$

Feature selection

Mixture models

Linear 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

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

$$\sum_{k=1}^K \frac{1}{(2\pi\beta_k)^{n/2}} \exp\left(-\frac{1}{2\beta_k}(\mathbf{y} - \mathbf{w}_k^\top \mathbf{X})^\top (\mathbf{y} - \mathbf{w}_k^\top \mathbf{X})\right).$$

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

To find maximum likelihood estimates of $\hat{\theta}$

$$\hat{\theta} = \arg \max_{\theta} \ln p(\mathbf{y}|\theta),$$

introduce hidden indicator variables $Z = [\mathbf{z}_1, \dots, \mathbf{z}_m]$, $z_{ik} \in \{0, 1\}$, such that

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

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

$$p(\mathbf{y}|X, Z, \theta) = \sum_{i=1}^m \sum_{k=1}^K z_{ik} (\ln \pi_k + \ln \mathcal{N}(y_i | \mathbf{w}_k^T \mathbf{x}_i, \beta)).$$

EM-algorithm: instead of $p(\mathbf{y}|X, \theta)$ maximize the expected loglikelihood $E_Z[p(\mathbf{y}, Z|X, \theta)]$ of the observed data.

Expectation step

Expectation-Maximization algorithm maximizes $E_Z[p(\mathbf{y}, Z|X, \theta)]$, updating parameters estimates $\theta^{(r+1)}$ in two iterative steps with $\theta^{(r)}$ fixed.

E-step: obtain $E(Z) = [\gamma_{ik}]$. Using Bayesian rule, obtain:

$$\gamma_{ik}^{(r+1)} = E(z_{ik}) = p(k|\mathbf{x}_i, \theta^{(r)}) = \frac{\pi_k \mathcal{N}(y_i | \mathbf{x}_i^T \mathbf{w}_k^{(r)}, \beta^{(r)})}{\sum_{k'=1}^K \pi_{k'} \mathcal{N}(y_i | \mathbf{x}_i^T \mathbf{w}_{k'}^{(r)}, \beta^{(r)})}.$$

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

$$Q^{(r)}(\theta) = E_Z(\ln p(\mathbf{y}, Z|\theta)) = \sum_{i=1}^m \sum_{k=1}^K \gamma_{ik}^{(r+1)} \left(\ln \pi_k^{(r)} + \ln \mathcal{N}(y_i | \mathbf{x}_i^T \mathbf{w}_k^{(r)}, \beta^{(r)}) \right)$$

Maximization step

Expectation-Maximization algorithm maximizes $E_Z[p(\mathbf{y}, Z|X, \theta)]$, updating parameters estimates $\theta^{(r+1)}$ in two iterative steps with $\theta^{(r)}$ fixed.

M-step: update parameters θ , maximizing $Q^{(r)}(\theta) = E_Z(\ln p(\mathbf{y}, Z|\theta))$ with respect to θ with $\gamma^{(r+1)}$ fixed:

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

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

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

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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

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

for $p(y|\mathbf{x}, \theta)$.

Here $p(k|\mathbf{x}, \theta)$ correspond to weight parameters π_k in mixture models dependent on the inputs \mathbf{x} :

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

Parameter's estimation via EM differs only in M-step.

EM for Mixture of experts

E-step: compute hidden variables $\gamma_{ik}^{(r+1)}$, the expectation of the indicator variables, as previously shown.

M-step: find new parameter estimates

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

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

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

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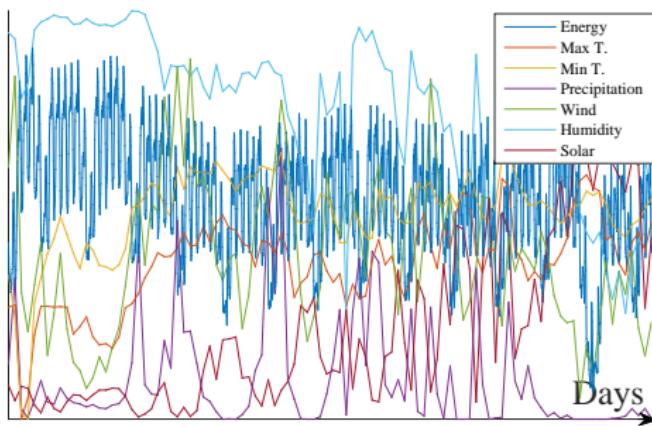
$$\mathbf{w}_k^{(r+1)} = \arg \max_{\mathbf{w}_k} \left[- \sum_{i=1}^m \gamma_{ik}^{(r+1)} (y_i - \mathbf{w}_k^\top \mathbf{x}_i)^2 \right],$$

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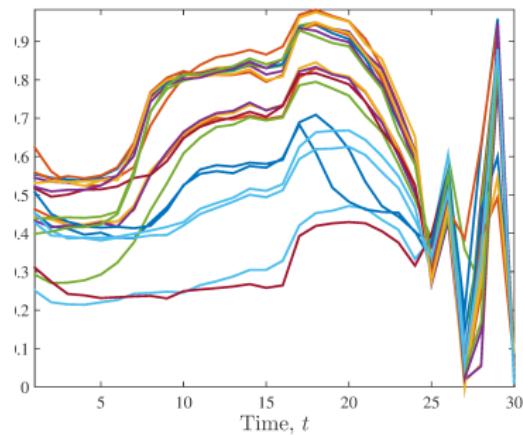
Computational experiments

Data

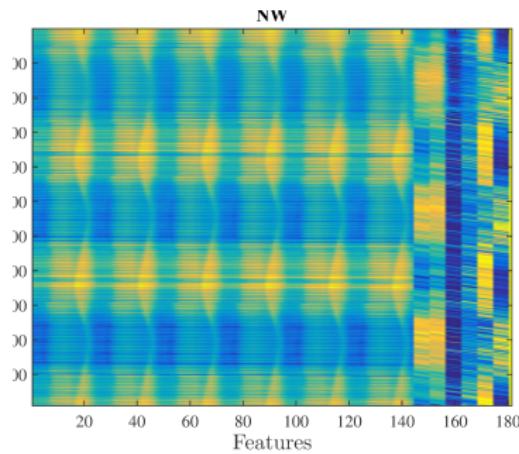
1. Original Polish electricity load time series, 1999–2004, including:
 - ▶ hourly energy time series (total of 52512 observations),
 - ▶ six daily weather time series from Warsaw (2188 observations): Max Temperature, Min Temperature, Precipitation, Wind, Relative Humidity, Solar.
- 2–5. Data sets with artificial inserted missing values, 1, 3, 5 and 10% missing.
6. Data set with artificially varied sampling rate.



Data



Target variables.



The design matrix.

Models and features

Models:

- ▶ Baseline method: $\hat{s}_i = s_{i-1}$.
- ▶ Multivariate linear regression (MLR) with l_2 -regularization.
Regularization coefficient: 2
- ▶ SVR with multiple output. Kernel type: RBF, $p_1: 2$, $p_2: 0$, $\gamma: 0.5$, $\lambda: 4$.
- ▶ Feed-forward ANN with single hidden layer, size: 25
- ▶ Random forest (RF). Number of trees: 25 , number of variables for each decision split: 48.

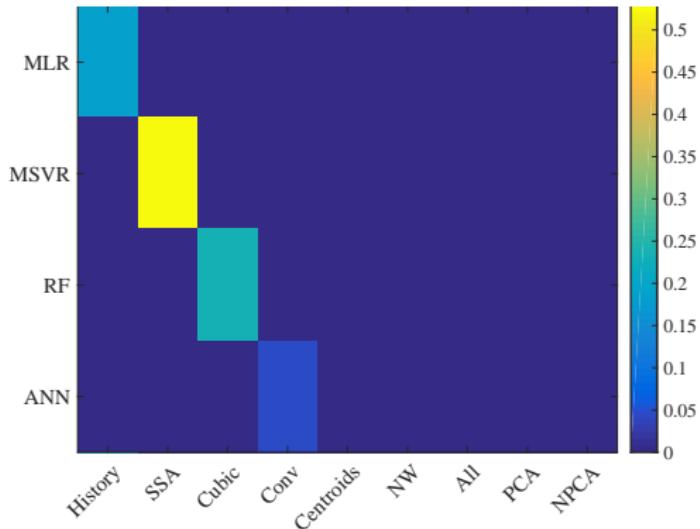
Feature combinations:

- ▶ History: the standard regression-based forecast with no additional features.
- ▶ SSA, Cubic, Conv, Centroids, NW: history + a particular feature.
- ▶ All: all of the above, with no feature selection.
- ▶ PCA and NPCA: all generation strategies with feature selection.

Forecasting errors, SMAPE

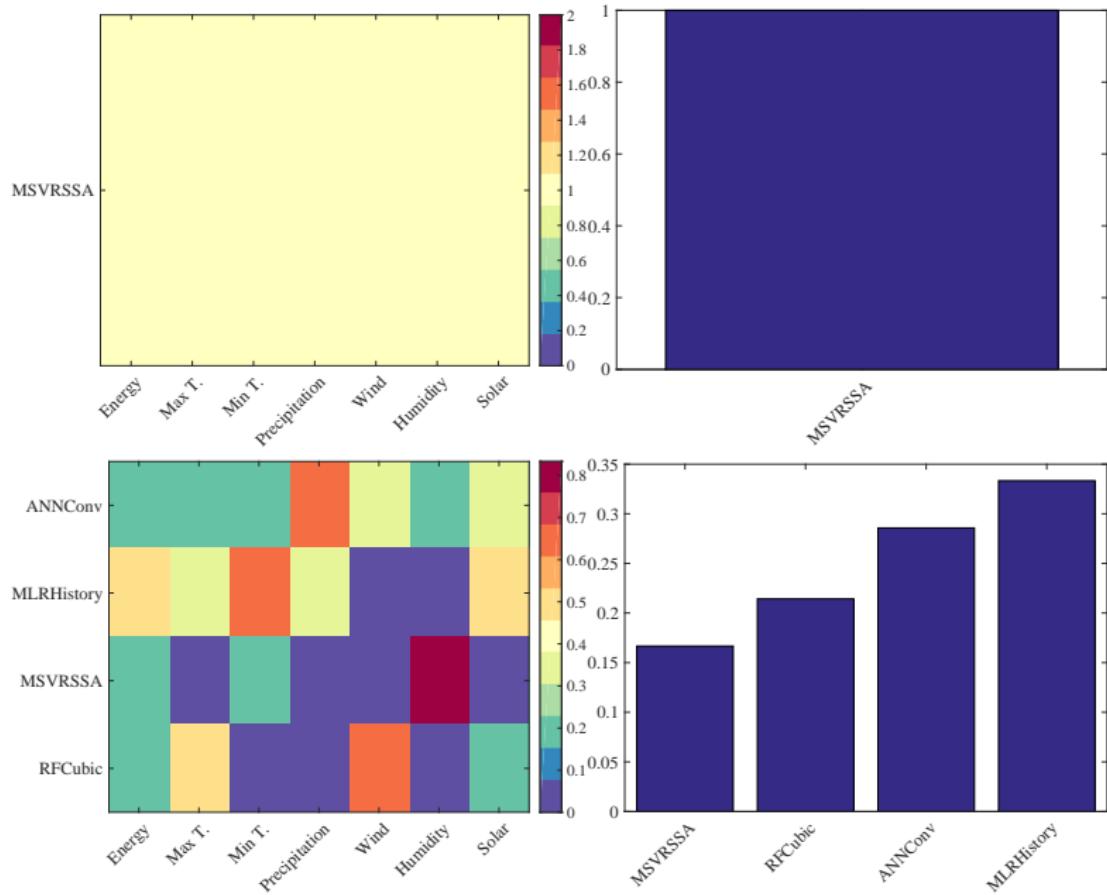
Data	Energy	Max T.	Min T.	Precip.	Wind	Humid.	Solar
Test							
orig	0.111	0.127	0.111	1.222	0.396	0.201	0.495
0.01	0.230	0.185	0.129	1.028	0.397	0.254	0.577
0.03	0.231	0.191	0.137	1.026	0.396	0.253	0.591
0.05	0.230	0.200	0.141	1.017	0.390	0.250	0.592
0.1	0.247	0.198	0.151	1.192	0.381	0.225	0.562
varying	0.124	0.139	0.102	1.232	0.395	0.219	0.489
Train							
orig	0.031	0.073	0.057	0.848	0.111	0.051	0.267
0.01	0.034	0.055	0.040	0.595	0.111	0.055	0.253
0.03	0.034	0.057	0.042	0.595	0.110	0.055	0.249
0.05	0.034	0.060	0.043	0.592	0.109	0.054	0.246
0.1	0.031	0.081	0.063	0.743	0.102	0.051	0.272
varying	0.027	0.057	0.044	0.888	0.112	0.055	0.272

Feature analysis

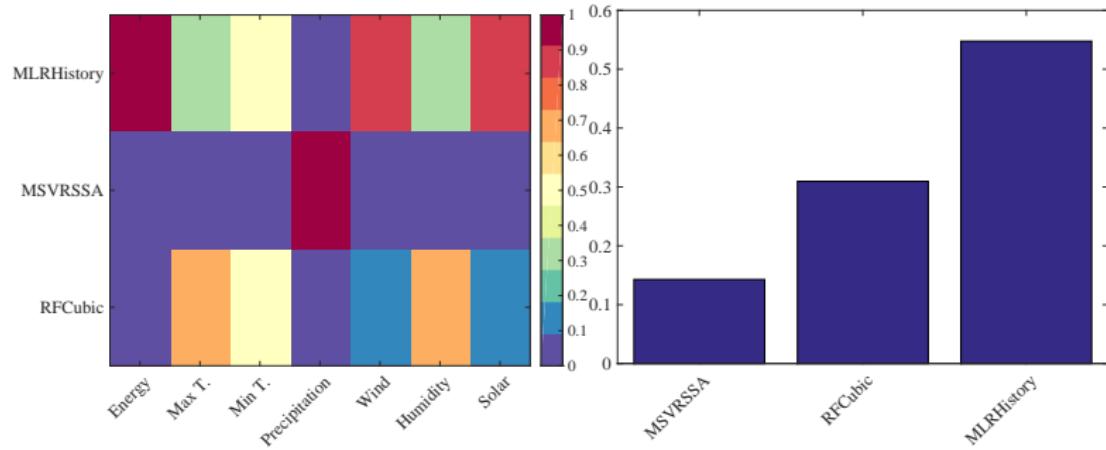
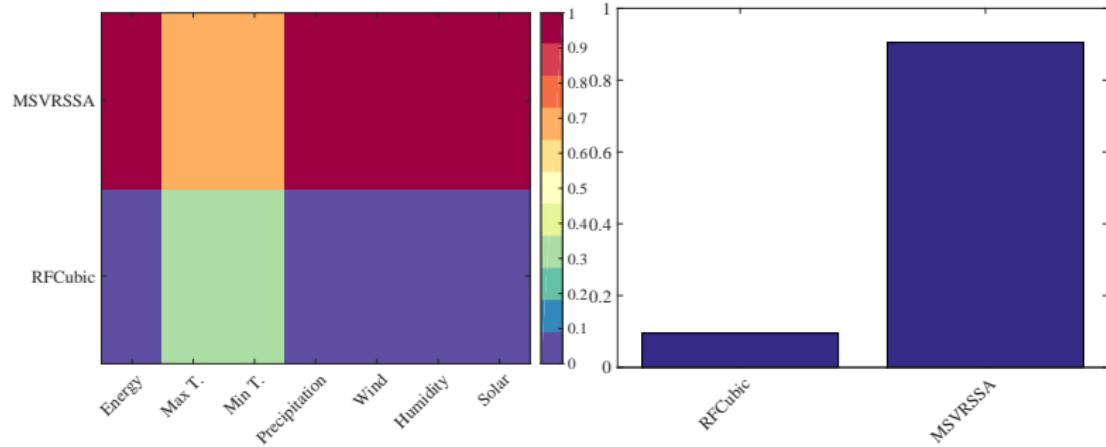


Ratio of times each combination of model and feature performed best for at least one of the time series (7) or error functions (6), all (6) data sets ($6 \times 7 \times 6 = 252$ cases).

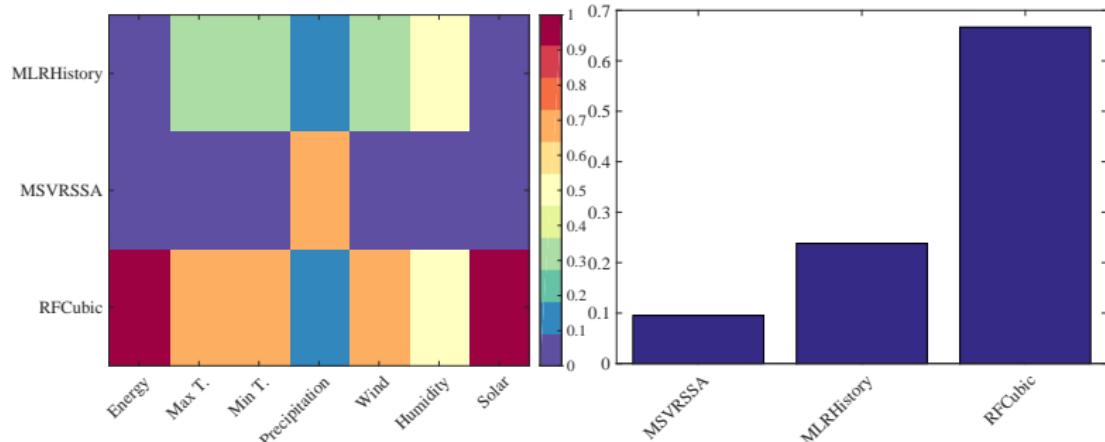
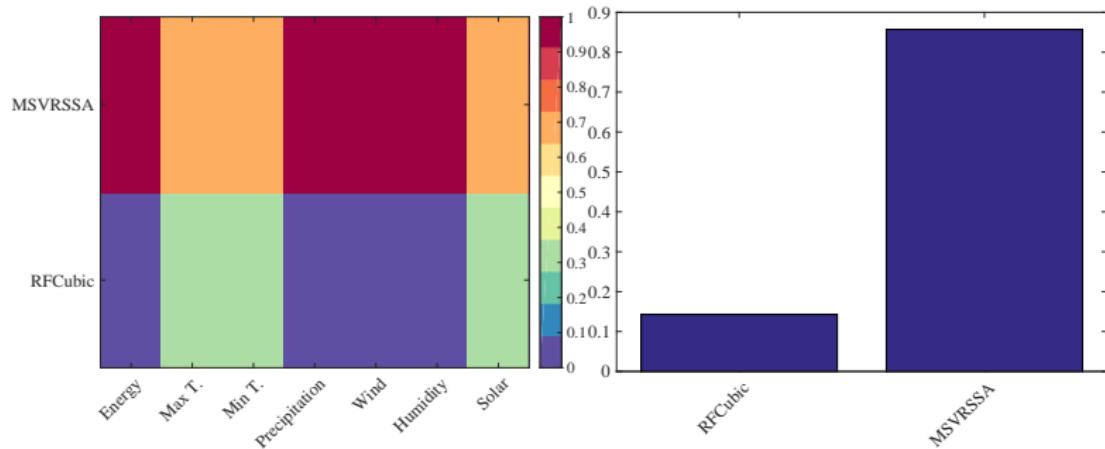
Best models, train/test residues



Best models, standard deviations (train/test residues)

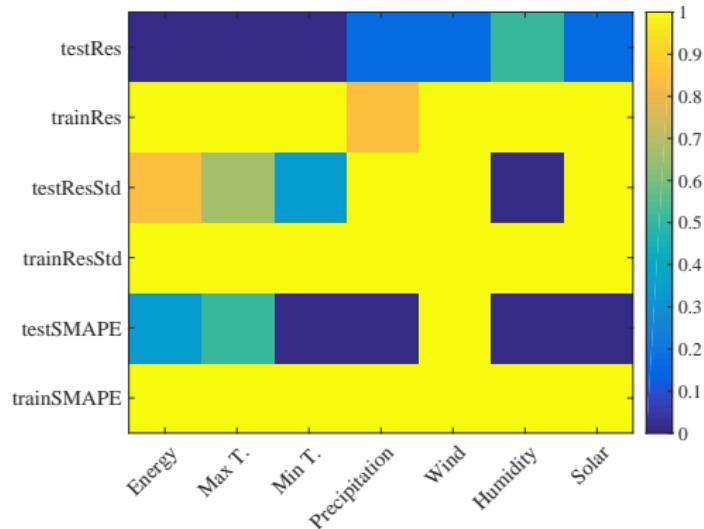


Best models, train/test SMAPE



Validation of multiple forecast approach

Additional loss functions: mean residues (test/train), standard deviation of residues (test/train) → 6 loss functions.



Ratio of datasets, where best forecasts outperformed baseline according to a particular error function.

Resampling time series

Resampling time series

Suppose that the observations $s_i = s(t_i)$ of the signal $s(t)$ are sampled unevenly:

$$G = \{t_1, \dots, t_T\}, \quad t_i \neq i \cdot \frac{t_T - t_1}{T - 1}$$

To obtain evenly spaced observations:

- 1) select a new sampling rate τ_{rs} ,
- 2) form the new grid

$$G_s = \{t_1, \dots, T_{rs}\}, \quad t_i = t_1 + (i - 1) \cdot \tau_{rs}$$

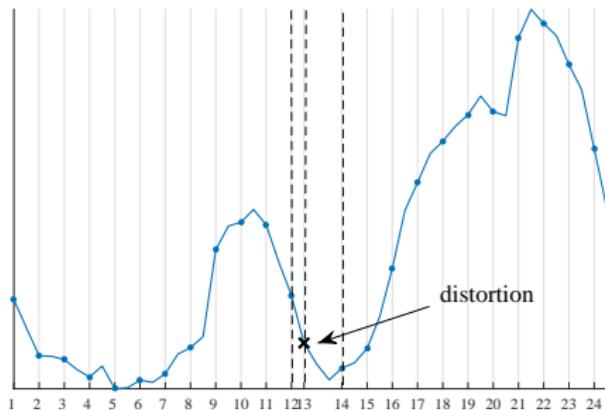
- 3) and approximate unobserved evenly-spaced values $\hat{s}_i = s(t_i)$, $t_i \in G_s$ using the sampled observations $s_i = s(t_i)$, $t_i \in G$.

Resampling: special case

1. The initial sampling rate is approximately even, but distortions are possible:

$$t_i = i \cdot \tau + \delta_i, |\delta_i| < \frac{\tau}{2}.$$

In this case the number T_s of resampled observations equals the initial number of observations T .

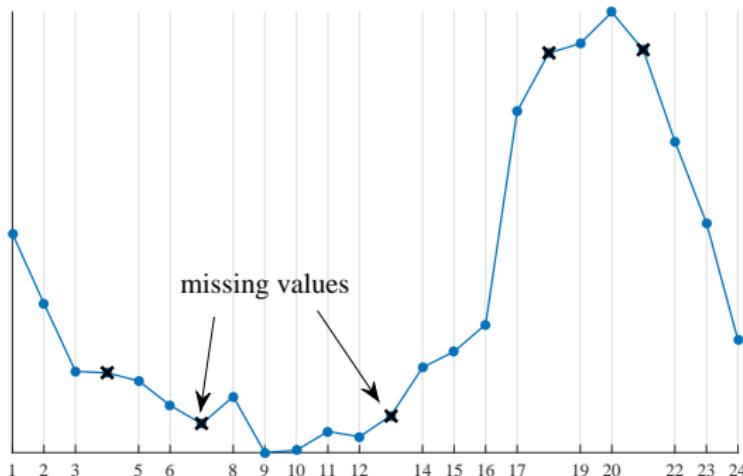


Resampling: special case

2. The sampling rate is even, but some values are missing:

$$|t_{i+1} - t_i| = n\tau, n \in \mathbb{N}.$$

Here $\tau_s = \tau$ and missing values are the only ones that one needs to approximate.

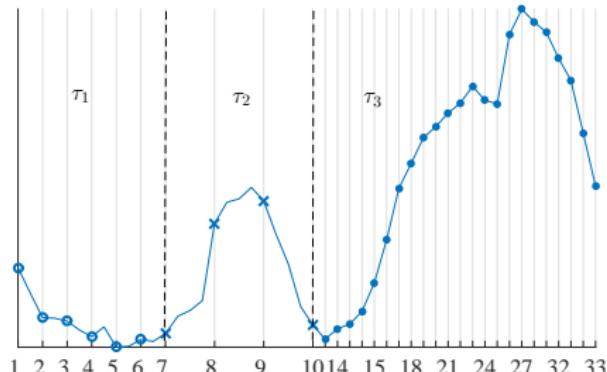


Resampling: special case

3. Time series \mathbf{s} comprises a finite number of intervals \mathbf{s}_k , each sampled from $s(t)$ at fixed sampling rate:

$$\mathbf{s} = \left[s(\tau_1), \dots, s(T_1\tau_1), s(T_1\tau_1 + \tau_2), \dots, s\left(\sum_k T_k\tau_k\right) \right],$$

where $\sum_k T_k = T$. Here we select the maximum sampling rate $f_s = \max_k \frac{1}{\tau_k}$ and upsample the rest time series, using piecewise constant approximation.



Resampling details

Suppose that the signal $s(t)$ is bandlimited with frequency f_b .

Nyquist–Shannon sampling condition: it is sufficient to sample the signal $s(t)$ with frequency

$$\frac{1}{\tau_{rs}} = f_s > 2f_b$$

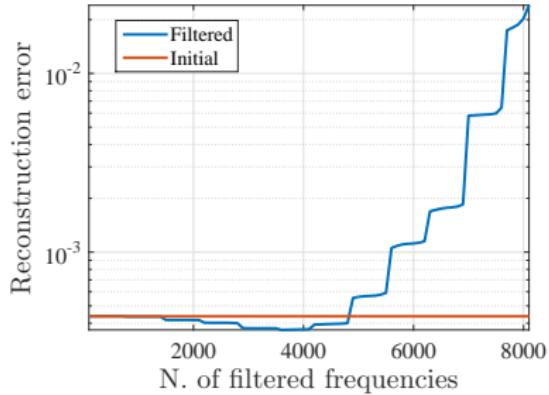
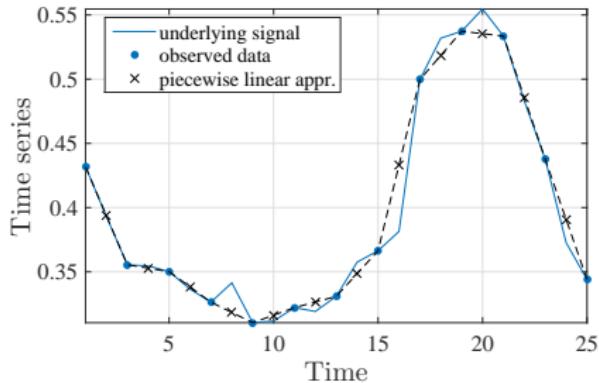
to be able to fully reconstruct the signal from its discretely sampled observations $s(t_i) = s(i\tau_s)$.

Discrete signals are never bandlimited \Rightarrow the time series have to be low-pass filtered to satisfy the Nyquist condition.

Upsampling procedure

Let G_s be the desired grid, $G \subseteq G_s$. To obtain $s(G_s)$:

1. Approximate $s(G_s \setminus G)$ using piecewise linear approximation.
2. Find s 's FFT coefficients a_j, b_j for $j = 1, \dots, 2^{\lfloor \log_2 T \rfloor}$.
3. Set $a_j = 0, b_j = 0$, for $j > 2^{\lfloor \log_2 T \rfloor - 1}$.
4. Reconstruct the time series, using inverse FFT.



Resampling

Piece-wise constant approximation of missing values:

