

Dimensionality Reduction for Signal Analysis

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Signal decoding problem

Goal

Investigate dependencies in both input and target spaces and build a stable model for signal decoding in the case of multicorrelated object description.

Challenge

- Measurements of spatial-temporal data are interacted since sensors are close to each other.
- Target variable is a vector whose elements are dependent.

Solution

Propose dimensionality reduction and feature selection algorithms which take into account dependencies in both input and target spaces.

Related works

- Katrutsa A., Strijov V. Comprehensive study of feature selection methods to solve multicollinearity problem according to evaluation criteria // *Expert Systems with Applications* 76, 2017.
- Li J. et al. Feature selection: A data perspective // *ACM Computing Surveys (CSUR)* 50(6), 2017.
- Eliseyev A. et al. Iterative N-way partial least squares for a binary self-paced brain-computer interface in freely moving animals // *Journal of neural engineering* 4(8), 2011.
- Rodriguez-Lujan I. et al. Quadratic programming feature selection // *Journal of Machine Learning Research* 11(Apr), 2010.
- Motrenko A., Strijov V. Multi-way Feature Selection for ECoG-based Brain-Computer Interface // *Expert Systems with Applications* Submitted to the journal.

Multivariate regression

Given

Dataset (\mathbf{X}, \mathbf{Y}) , design matrix $\mathbf{X} \in \mathbb{R}^{m \times n}$, target matrix $\mathbf{Y} \in \mathbb{R}^{m \times r}$,

$$\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n]; \quad \mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_r].$$

Model

Forecast a dependent variable $\mathbf{y} \in \mathbb{R}^r$ from an independent input object $\mathbf{x} \in \mathbb{R}^n$

$$\mathbf{y} = \mathbf{\Theta} \mathbf{x} + \boldsymbol{\varepsilon}, \quad \mathbf{\Theta} \in \mathbb{R}^{r \times n}.$$

Loss function

$$\mathcal{L}(\mathbf{\Theta} | \mathbf{X}, \mathbf{Y}) = \left\| \underset{m \times r}{\mathbf{Y}} - \underset{m \times n}{\mathbf{X}} \cdot \underset{r \times n}{\mathbf{\Theta}^T} \right\|_2^2 \rightarrow \min_{\mathbf{\Theta}}.$$
$$\mathbf{\Theta}^T = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}.$$

The linear dependent columns of the matrix \mathbf{X} leads to an instable solution. To avoid the strong linear dependence, dimensionality reduction and feature selection techniques are used.

Dimensionality reduction

Goal

- project the matrices \mathbf{X} and \mathbf{Y} into joint latent space;
- maximize covariance between the projections;
- save variance of the initial matrices.

Partial Least Squares (PLS) regression

$$\mathbf{X}_{m \times n} = \mathbf{T}_{m \times l} \cdot \mathbf{P}_{l \times n}^T + \mathbf{F}_{m \times n} = \sum_{k=1}^l \mathbf{t}_k \cdot \mathbf{p}_k^T + \mathbf{F},$$

$$\mathbf{Y}_{m \times r} = \mathbf{U}_{m \times l} \cdot \mathbf{Q}_{l \times r}^T + \mathbf{E}_{m \times r} = \sum_{k=1}^l \mathbf{u}_k \cdot \mathbf{q}_k^T + \mathbf{E}.$$

$$\mathbf{U} \approx \mathbf{T}\mathbf{B}, \quad \mathbf{B} = \text{diag}(\beta_k), \quad \beta_k = \mathbf{u}_k^T \mathbf{t}_k / (\mathbf{t}_k^T \mathbf{t}_k).$$

PLS pseudocode

Require: $\mathbf{X}, \mathbf{Y}, l$;

Ensure: $\mathbf{T}, \mathbf{P}, \mathbf{Q}$;

- 1: normalize matrices \mathbf{X} и \mathbf{Y} by columns
- 2: initialize \mathbf{u}_0 (the first column of \mathbf{Y})
- 3: $\mathbf{X}_1 = \mathbf{X}; \mathbf{Y}_1 = \mathbf{Y}$
- 4: **for** $k = 1, \dots, l$ **do**
- 5: **repeat**
- 6: $\mathbf{w}_k := \mathbf{X}_k^\top \mathbf{u}_{k-1} / (\mathbf{u}_{k-1}^\top \mathbf{u}_{k-1}); \quad \mathbf{w}_k := \frac{\mathbf{w}_k}{\|\mathbf{w}_k\|}$
- 7: $\mathbf{t}_k := \mathbf{X}_k \mathbf{w}_k$
- 8: $\mathbf{c}_k := \mathbf{Y}_k^\top \mathbf{t}_k / (\mathbf{t}_k^\top \mathbf{t}_k); \quad \mathbf{c}_k := \frac{\mathbf{c}_k}{\|\mathbf{c}_k\|}$
- 9: $\mathbf{u}_k := \mathbf{Y}_k \mathbf{c}_k$
- 10: **until** \mathbf{t}_k stabilizes
- 11: $\mathbf{p}_k := \mathbf{X}_k^\top \mathbf{t}_k / (\mathbf{t}_k^\top \mathbf{t}_k), \quad \mathbf{q}_k := \mathbf{Y}_k^\top \mathbf{t}_k / (\mathbf{t}_k^\top \mathbf{t}_k)$
- 12: $\mathbf{X}_{k+1} := \mathbf{X}_k - \mathbf{t}_k \mathbf{p}_k^\top$
- 13: $\mathbf{Y}_{k+1} := \mathbf{Y}_k - \mathbf{t}_k \mathbf{q}_k^\top$

PLS regression

Statement (Isachenko, 2017)

The best description of the matrices \mathbf{X} and \mathbf{Y} taking into account their interrelation is achieved by maximization of the covariance between the vectors \mathbf{t}_k and \mathbf{u}_k .

Statement (Isachenko, 2017)

The vector \mathbf{w}_k and \mathbf{c}_k are eigenvectors of the matrices $\mathbf{X}_k^T \mathbf{Y}_k \mathbf{Y}_k^T \mathbf{X}_k$ and $\mathbf{Y}_k^T \mathbf{X}_k \mathbf{X}_k^T \mathbf{Y}_k$, corresponding to the maximum eigenvalues.

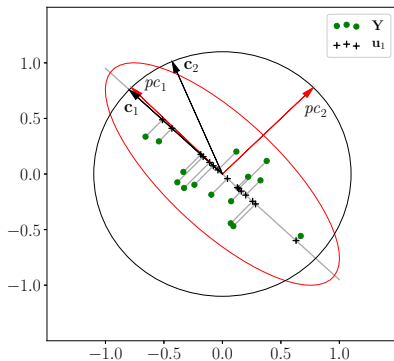
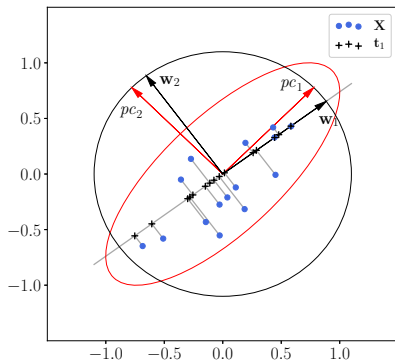
Statement (Isachenko, 2017)

The update rule for the vectors in steps (6)–(9) corresponds to the maximization of the covariance between the vectors \mathbf{t}_k and \mathbf{u}_k .

PLS regression model

$$\mathbf{Y} = \mathbf{UQ}^T + \mathbf{E} \approx \mathbf{TBQ}^T + \mathbf{E} = \mathbf{XW}^* \mathbf{BQ}^T + \mathbf{E} = \mathbf{X}\boldsymbol{\Theta} + \mathbf{E}.$$
$$\boldsymbol{\Theta} = \mathbf{W}(\mathbf{P}^T \mathbf{W})^{-1} \mathbf{BQ}^T, \quad \mathbf{T} = \mathbf{XW}^*, \quad \text{where } \mathbf{W}^* = \mathbf{W}(\mathbf{P}^T \mathbf{W})^{-1}.$$

PLS example for two-dimensional case



Feature selection problem

Goal

Find a boolean vector $\mathbf{a} = \{0, 1\}^n$ of indicators for selected features.

Feature selection error function

$$\mathbf{a} = \arg \min_{\mathbf{a}' \in \{0, 1\}^n} S(\mathbf{a}' | \mathbf{X}, \mathbf{Y}).$$

Relaxed problem

From discrete domain $\{0, 1\}^n$ to continuous relaxation $[0, 1]^n$:

$$\mathbf{z} = \arg \min_{\mathbf{z}' \in [0, 1]^n} S(\mathbf{z}' | \mathbf{X}, \mathbf{Y}), \quad a_j = [z_j > \tau].$$

Once the solution \mathbf{a} is known:

$$\mathcal{L}(\Theta_{\mathbf{a}} | \mathbf{X}_{\mathbf{a}}, \mathbf{Y}) = \left\| \mathbf{Y} - \mathbf{X}_{\mathbf{a}} \Theta_{\mathbf{a}}^T \right\|_2^2 \rightarrow \min_{\Theta_{\mathbf{a}}},$$

where the subscript \mathbf{a} indicates the submatrix with the columns for which $a_j = 1$.

Quadratic Programming Feature Selection

$$\|\boldsymbol{\nu} - \mathbf{X}\boldsymbol{\theta}\|_2^2 \rightarrow \min_{\boldsymbol{\theta} \in \mathbb{R}^n}.$$

Quadratic programming problem

$$S(\mathbf{z}|\mathbf{X}, \boldsymbol{\nu}) = (1 - \alpha) \cdot \underbrace{\mathbf{z}^T \mathbf{Q} \mathbf{z}}_{\text{Sim}(\mathbf{X})} - \alpha \cdot \underbrace{\mathbf{b}^T \mathbf{z}}_{\text{Rel}(\mathbf{X}, \boldsymbol{\nu})} \rightarrow \min_{\substack{\mathbf{z} \geq \mathbf{0}_n \\ \mathbf{1}_n^T \mathbf{z} = 1}}.$$

- $\mathbf{z} \in [0, 1]^n$ – feature importances;
- $\mathbf{Q} \in \mathbb{R}^{n \times n}$ – pairwise feature similarities;
- $\mathbf{b} \in \mathbb{R}^n$ – feature relevances to the target vector.

$$\mathbf{Q} = [|\text{corr}(\chi_i, \chi_j)|]_{i,j=1}^n, \quad \mathbf{b} = [|\text{corr}(\chi_i, \boldsymbol{\nu})|]_{i=1}^n.$$

Statement

In the case of semidefinite matrix \mathbf{Q} the QPFS problem is convex. Shift spectrum for semidefinite relaxation:

$$\mathbf{Q} \rightarrow \mathbf{Q} - \lambda_{\min} \mathbf{I}.$$

Multivariate QPFS

Relevance Aggregation (RelAgg)

$$\mathbf{b} = [|\text{corr}(\chi_i, \nu)|]_{i=1}^n \rightarrow \mathbf{b} = \left[\sum_{k=1}^r |\text{corr}(\chi_i, \nu_k)| \right]_{i=1}^n.$$

Drawback: the approach does not use the dependencies in the columns of \mathbf{Y} .

Symmetric Importances (SymImp)

Penalize correlated targets by $\text{Sim}(\mathbf{Y})$

$$\alpha_1 \cdot \underbrace{\mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x}_{\text{Sim}(\mathbf{X})} - \alpha_2 \cdot \underbrace{\mathbf{z}_x^T \mathbf{B} \mathbf{z}_y}_{\text{Rel}(\mathbf{X}, \mathbf{Y})} + \alpha_3 \cdot \underbrace{\mathbf{z}_y^T \mathbf{Q}_y \mathbf{z}_y}_{\text{Sim}(\mathbf{Y})} \rightarrow \min_{\substack{\mathbf{z}_x \geq \mathbf{0}_n, \mathbf{1}_n^T \mathbf{z}_x = 1 \\ \mathbf{z}_y \geq \mathbf{0}_r, \mathbf{1}_r^T \mathbf{z}_y = 1}}.$$

$$\mathbf{Q}_x = [|\text{corr}(\chi_i, \chi_j)|]_{i,j=1}^n, \mathbf{Q}_y = [|\text{corr}(\nu_i, \nu_j)|]_{i,j=1}^r, \mathbf{B} = [|\text{corr}(\chi_i, \nu_j)|]_{i=1, \dots, n, j=1, \dots, r}.$$

$$\alpha_1 + \alpha_2 + \alpha_3 = 1, \quad \alpha_i \geq 0.$$

Multivariate QPFS

SymImp penalizes targets that are correlated and are explained by features to a lesser extent.

$$\underbrace{\alpha_1 \cdot \mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x}_{\text{Sim}(\mathbf{X})} - \underbrace{\alpha_2 \cdot \mathbf{z}_x^T \mathbf{B} \mathbf{z}_y}_{\text{Rel}(\mathbf{X}, \mathbf{Y})} \rightarrow \min_{\substack{\mathbf{z}_x \geq \mathbf{0}_n \\ \mathbf{1}_n^T \mathbf{z}_x = 1}} ; \quad \underbrace{\alpha_3 \cdot \mathbf{z}_y^T \mathbf{Q}_y \mathbf{z}_y}_{\text{Sim}(\mathbf{Y})} + \underbrace{\alpha_2 \cdot \mathbf{z}_x^T \mathbf{B} \mathbf{z}_y}_{\text{Rel}(\mathbf{X}, \mathbf{Y})} \rightarrow \min_{\substack{\mathbf{z}_y \geq \mathbf{0}_r \\ \mathbf{1}_r^T \mathbf{z}_y = 1}} .$$

Minimax approach (MinMax)

$$\min_{\substack{\mathbf{z}_x \geq \mathbf{0}_n \\ \mathbf{1}_n^T \mathbf{z}_x = 1}} \max_{\substack{\mathbf{z}_y \geq \mathbf{0}_r \\ \mathbf{1}_r^T \mathbf{z}_y = 1}} \left(\text{or } \max_{\substack{\mathbf{z}_y \geq \mathbf{0}_r \\ \mathbf{1}_r^T \mathbf{z}_y = 1}} \min_{\substack{\mathbf{z}_x \geq \mathbf{0}_n \\ \mathbf{1}_n^T \mathbf{z}_x = 1}} \right) \left[\underbrace{\alpha_1 \cdot \mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x}_{\text{Sim}(\mathbf{X})} - \underbrace{\alpha_2 \cdot \mathbf{z}_x^T \mathbf{B} \mathbf{z}_y}_{\text{Rel}(\mathbf{X}, \mathbf{Y})} - \underbrace{\alpha_3 \cdot \mathbf{z}_y^T \mathbf{Q}_y \mathbf{z}_y}_{\text{Sim}(\mathbf{Y})} \right] .$$

Theorem (Isachenko, 2018)

For positive definite matrices \mathbf{Q}_x and \mathbf{Q}_y the maxmin and minmax problems have the same optimal value.

Theorem (Isachenko, 2018)

Minimax problem is equivalent to the quadratic problem with $n + r + 1$ variables.

Shift spectrum to obtain the convex semidefinite relaxation.

Multivariate QPFS

Maximum Relevances (MaxRel)

$$\min_{\substack{\mathbf{z}_x \geq \mathbf{0}_n \\ \mathbf{1}_n^T \mathbf{z}_x = 1}} \max_{\substack{\mathbf{z}_y \geq \mathbf{0}_r \\ \mathbf{1}_r^T \mathbf{z}_y = 1}} \left[(1 - \alpha) \cdot \mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x - \alpha \cdot \mathbf{z}_x^T \mathbf{B} \mathbf{z}_y \right].$$

Theorem (Isachenko, 2018)

For positive definite matrices \mathbf{Q}_x the max-min and min-max problems have the same optimal value and the final quadratic problem is convex.

Assymmetric importances (AsymImp)

$$\underbrace{\alpha_1 \cdot \mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x}_{\text{Sim}(\mathbf{X})} - \underbrace{\alpha_2 \cdot \left(\mathbf{z}_x^T \mathbf{B} \mathbf{z}_y - \mathbf{b}^T \mathbf{z}_y \right)}_{\text{Rel}(\mathbf{X}, \mathbf{Y})} + \underbrace{\alpha_3 \cdot \mathbf{z}_y^T \mathbf{Q}_y \mathbf{z}_y}_{\text{Sim}(\mathbf{Y})} \rightarrow \min_{\substack{\mathbf{z}_x \geq \mathbf{0}_n, \mathbf{1}_n^T \mathbf{z}_x = 1 \\ \mathbf{z}_y \geq \mathbf{0}_r, \mathbf{1}_r^T \mathbf{z}_y = 1}}.$$

For $b_j = \max_{i=1, \dots, n} [\mathbf{B}]_{i,j}$ coefficients of \mathbf{z}_y in $\text{Rel}(\mathbf{X}, \mathbf{Y})$ are non-negative.

Statement

For the univariate case $r = 1$ the proposed strategies SymImp, MinMax, MaxRel, AsymImp coincide with the original QPFS algorithm.

Summary of the proposed algorithms

Algorithm	Problem	Error function $S(\mathbf{z} \mathbf{X}, \mathbf{Y})$
RelAgg	$\min [\text{Sim}(\mathbf{X}) - \text{Rel}(\mathbf{X}, \mathbf{Y})]$	$\min_{\mathbf{z}_x} [(1 - \alpha) \cdot \mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x - \alpha \cdot \mathbf{z}_x^T \mathbf{B} \mathbf{1}_r]$
SymImp	$\min [\text{Sim}(\mathbf{X}) - \text{Rel}(\mathbf{X}, \mathbf{Y}) + \text{Sim}(\mathbf{Y})]$	$\min_{\mathbf{z}_x, \mathbf{z}_y} [\alpha_1 \cdot \mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x - \alpha_2 \cdot \mathbf{z}_x^T \mathbf{B} \mathbf{z}_y + \alpha_3 \cdot \mathbf{z}_y^T \mathbf{Q}_y \mathbf{z}_y]$
MinMax	$\min [\text{Sim}(\mathbf{X}) - \text{Rel}(\mathbf{X}, \mathbf{Y})]$ $\max [\text{Rel}(\mathbf{X}, \mathbf{Y}) + \text{Sim}(\mathbf{Y})]$	$\min_{\mathbf{z}_x} \max_{\mathbf{z}_y} [\alpha_1 \cdot \mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x - \alpha_2 \cdot \mathbf{z}_x^T \mathbf{B} \mathbf{z}_y - \alpha_3 \cdot \mathbf{z}_y^T \mathbf{Q}_y \mathbf{z}_y]$
MaxRel	$\min [\text{Sim}(\mathbf{X}) - \text{Rel}(\mathbf{X}, \mathbf{Y})]$ $\max [\text{Rel}(\mathbf{X}, \mathbf{Y})]$	$\min_{\mathbf{z}_x} \max_{\mathbf{z}_y} [(1 - \alpha) \cdot \mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x - \alpha \cdot \mathbf{z}_x^T \mathbf{B} \mathbf{z}_y]$
AsymImp	$\min [\text{Sim}(\mathbf{X}) - \text{Rel}(\mathbf{X}, \mathbf{Y})]$ $\max [\text{Rel}(\mathbf{X}, \mathbf{Y}) + \text{Sim}(\mathbf{Y})]$	$\min_{\mathbf{z}_x, \mathbf{z}_y} [\alpha_1 \mathbf{z}_x^T \mathbf{Q}_x \mathbf{z}_x - \alpha_2 (\mathbf{z}_x^T \mathbf{B} \mathbf{z}_y - \mathbf{b}^T \mathbf{z}_y) + \alpha_3 \mathbf{z}_y^T \mathbf{Q}_y \mathbf{z}_y]$

Quality criteria

Scaled RMSE

Prediction quality:

$$\text{sRMSE}(\mathbf{Y}, \hat{\mathbf{Y}}_a) = \sqrt{\frac{\text{MSE}(\mathbf{Y}, \hat{\mathbf{Y}}_a)}{\text{MSE}(\mathbf{Y}, \bar{\mathbf{Y}})}} = \frac{\|\mathbf{Y} - \hat{\mathbf{Y}}_a\|_2}{\|\mathbf{Y} - \bar{\mathbf{Y}}\|_2}, \quad \text{where } \hat{\mathbf{Y}}_a = \mathbf{X}_a \boldsymbol{\Theta}_a^T.$$

$\bar{\mathbf{Y}}$ is a constant prediction.

Multicorrelation

Mean value of multiple correlation coefficient:

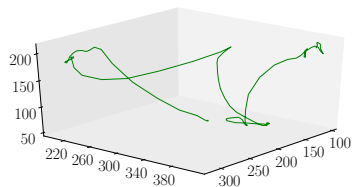
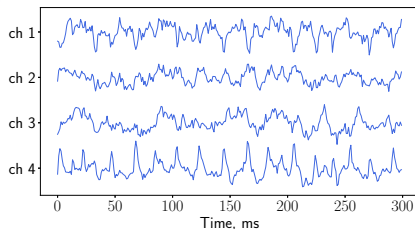
$$R^2 = \frac{1}{r} \text{tr} \left(\mathbf{C}^T \mathbf{R}^{-1} \mathbf{C} \right); \quad \mathbf{C} = [\text{corr}(\chi_i, \nu_j)]_{\substack{i=1, \dots, n, \\ j=1, \dots, r}}, \quad \mathbf{R} = [\text{corr}(\chi_i, \chi_j)]_{i,j=1}^n.$$

BIC

Bayesian Information Criteria is a trade-off between prediction quality and the number of selected features $\|\mathbf{a}\|_0$:

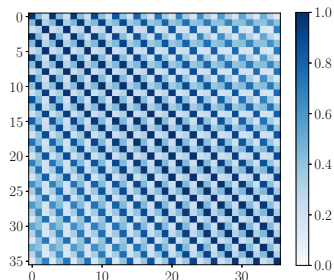
$$\text{BIC} = m \ln \left(\text{MSE}(\mathbf{Y}, \hat{\mathbf{Y}}_a) \right) + \|\mathbf{a}\|_0 \cdot \log m.$$

Computational experiment



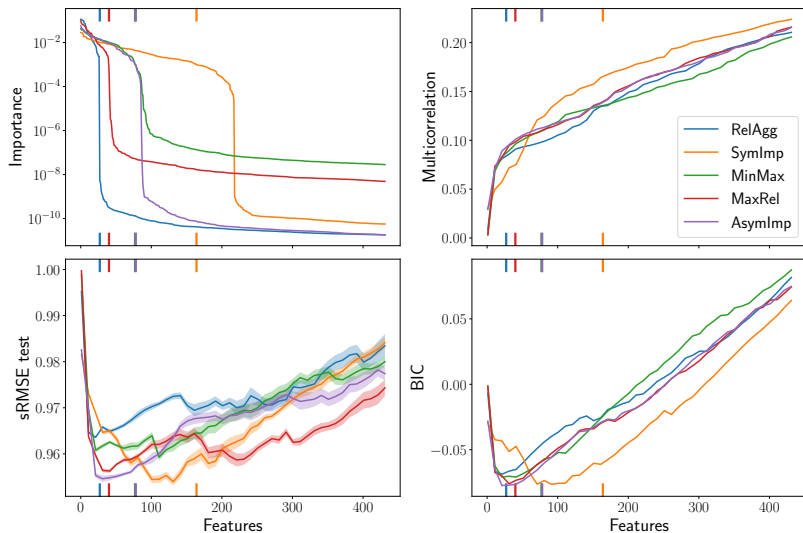
$$\mathbf{X} \in \mathbb{R}^{m \times (32 \cdot 27)}; \quad \mathbf{Y} \in \mathbb{R}^{m \times 3k}.$$

$$\mathbf{Y} = \begin{pmatrix} x_1 & y_1 & z_1 & \dots & x_k & y_k & z_k \\ x_2 & y_2 & z_2 & \dots & x_{k+1} & y_{k+1} & z_{k+1} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ x_m & y_m & z_m & \dots & x_{m+k} & y_{m+k} & z_{m+k} \end{pmatrix}$$



Y correlation matrix

Quality criteria evaluation



Stability of selected feature subsets

Experiment design

- generate bootstrap data

$$(\mathbf{X}, \mathbf{Y}) \rightarrow \{(\mathbf{X}_1, \mathbf{Y}_1), \dots, (\mathbf{X}_s, \mathbf{Y}_s)\};$$

- solve feature selection problem

$$\{(\mathbf{X}_1, \mathbf{Y}_1), \dots, (\mathbf{X}_s, \mathbf{Y}_s)\} \rightarrow \{\mathbf{z}_1, \dots, \mathbf{z}_s\};$$

- calculate statistics

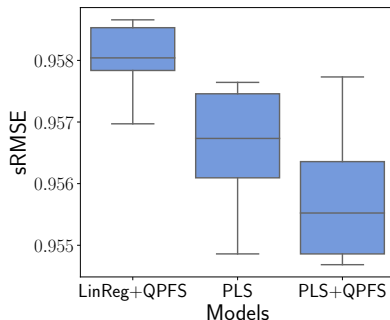
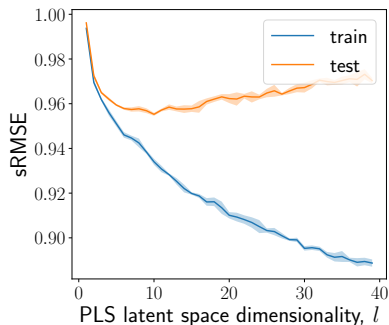
$$\{\mathbf{z}_1, \dots, \mathbf{z}_s\} \rightarrow \{\text{RMSE}, \|\mathbf{a}\|_0, \text{Spearman } \rho, \ell_2 \text{ dist}\}.$$

	sRMSE	$\ \mathbf{a}\ _0$	Spearman ρ	ℓ_2 dist
RelAgg	0.965 ± 0.002	26.8 ± 3.8	0.915 ± 0.016	0.145 ± 0.018
SymImp	0.961 ± 0.001	224.4 ± 9.0	0.910 ± 0.017	0.025 ± 0.002
MinMax	0.961 ± 0.002	101.0 ± 2.1	0.932 ± 0.009	0.059 ± 0.004
MaxRel	0.958 ± 0.003	41.2 ± 5.2	0.862 ± 0.027	0.178 ± 0.010
AsymImp	0.955 ± 0.001	85.8 ± 10.2	0.926 ± 0.011	0.078 ± 0.007

QPFS vs PLS

Design of experiment

To compare feature selection and dimensionality reduction for linear regression and PLS regression models.



Results

- The problem of ECoG signal decoding in high dimensional spaces is investigated.
- Dimensionality reduction technique with space structure analysis is investigated.
- Feature selection methods which take into account structure of both input and target spaces are proposed.
- The combination of feature selection and dimensionality reduction is proposed.
- Proposed feature selection algorithms give the stable and adequate solutions.

Conclusion

Publications

- Isachenko R., Strijov V. Metric learning for time series multiclass classification *Informatics and Applications*, 10(2), 2016.
- Isachenko R. et al. Feature Generation for Physical Activity Classification. *Artificial Intelligence and Decision Making*, 2018, submitted to the journal.
- Isachenko R., Strijov V. Quadratic programming optimization for Newton method. *Lobachevskii Journal of Mathematics*, 2018, accepted to the journal.
- Isachenko R., Strijov V. Dimensionality reduction for multivariate ECoG-based data. *Chemometrics*, 2018, ready for submission.

Conferences

- Lomonosov, 2016, Moscow. Metric learning in multiclass time series classification.
- Intelligent Data Processing Conference, 2016, Barcelona. Multimodel forecasting multiscale time series in internet of things.
- MMRO, 2017, Taganrog. Local models for classification of complex structured objects.