Feature selection and data dependencies analysis:
an operative tool for geospatial data,

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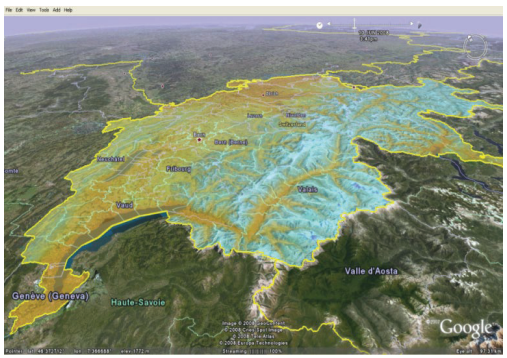
Motivation

Environmental sciences and geomatics are experiencing a previously unseen growth of data collection and storage (big data). This results in **High Dimensional** *feature spaces*.

Typical real data case studies:

- Wind fields $> 13d$
- Avalanches $> 40d$
- Landslides $> 18d$
- Permafrost $> 20d$
- Wildfires $> 25d$
- City pollution $> 50d$
- Remote sensing $> 100d$
- ...



Why Feature Selection?

Strongly relevant

Features that cannot be removed without affecting the original conditional target distribution

Weakly relevant, but not redundant

Features that can become necessary under certain condition

Weakly relevant and redundant

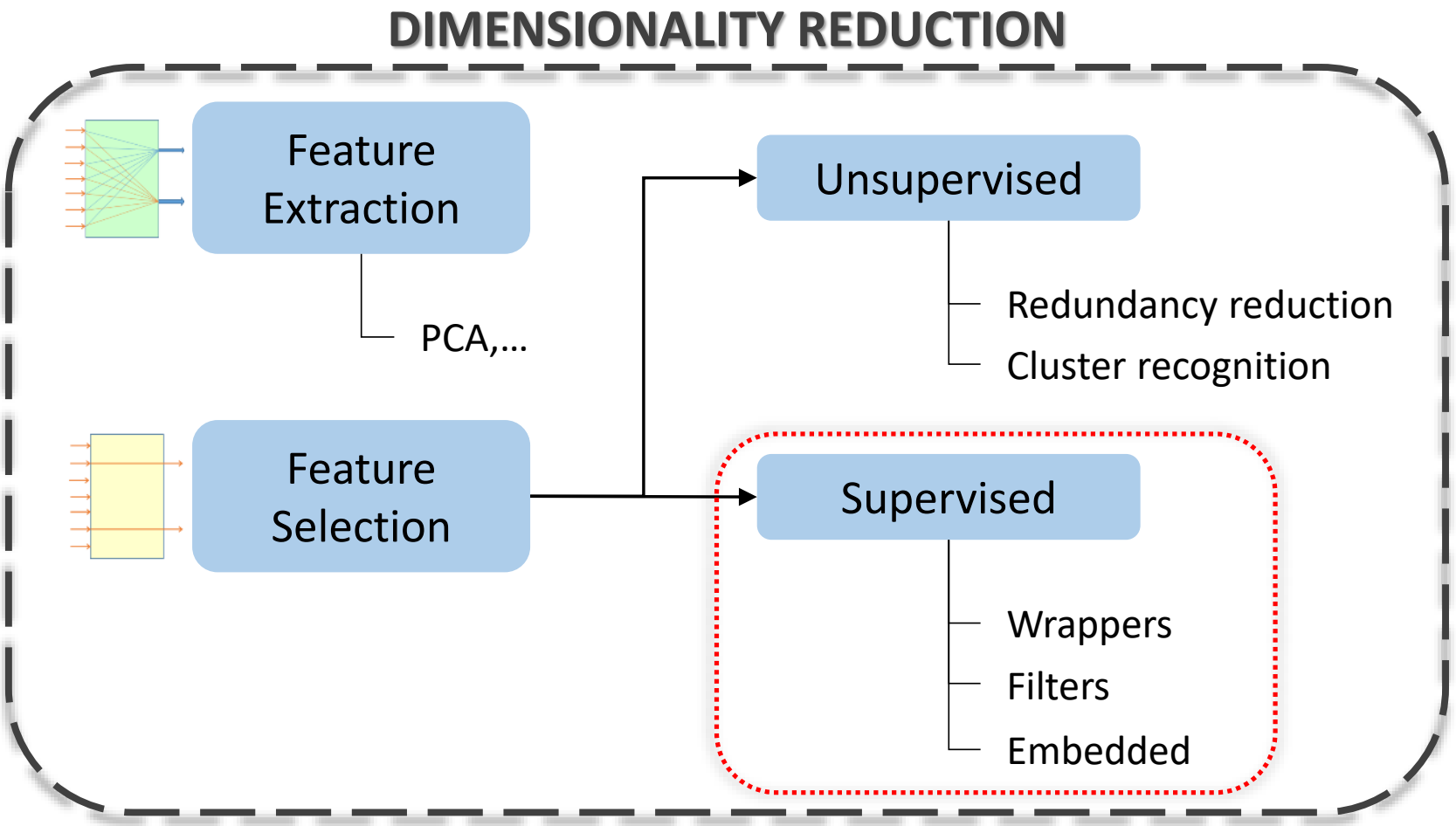
Features that can be completely replaced with a set of other features such that the target distribution is not disturbed

Irrelevant

Features which absence does not affect original conditional target distribution

- **Curse of dimensionality**: redundant or irrelevant features reduce the accuracy of prediction

From dimensionality reduction to feature selection



Wrappers

- Use the performance of a learning algorithm to determine the quality of the selected subset of feature
- With exhaustive search there are $2^p - 1$ models resulting from p-dimensional input space:
  - p $= 8 --> 255$ possible subsets
  - p $= 20 --> 1048575$ possible subsets
  - p $= 50 --> 1125899906842623$ possible subsets!!
- In most cases the exhaustive search is not computationally feasible. Several search strategies have been proposed, such as the sequential forward selection, the sequential backward selection, the randomized search...
- High computational time, high accuracy

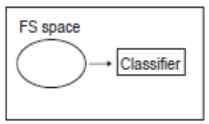
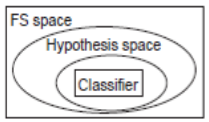
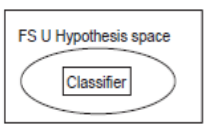
Filters

- Use the intrinsic characteristics in data to rank features using dependency, distance or consistency measures
- Many filters have been proposed in literature (ReliefF, Correlation-based FS, ...)
- Faster than, but not as accurate as, wrappers

Embedded

- Integrate feature selection in the learning process itself (e.g. Lasso, Ridge, Random Forest - but not really -, ...)
- Depending on the algorithm there may be a strong bias

Different methods, different advantages and disadvantages

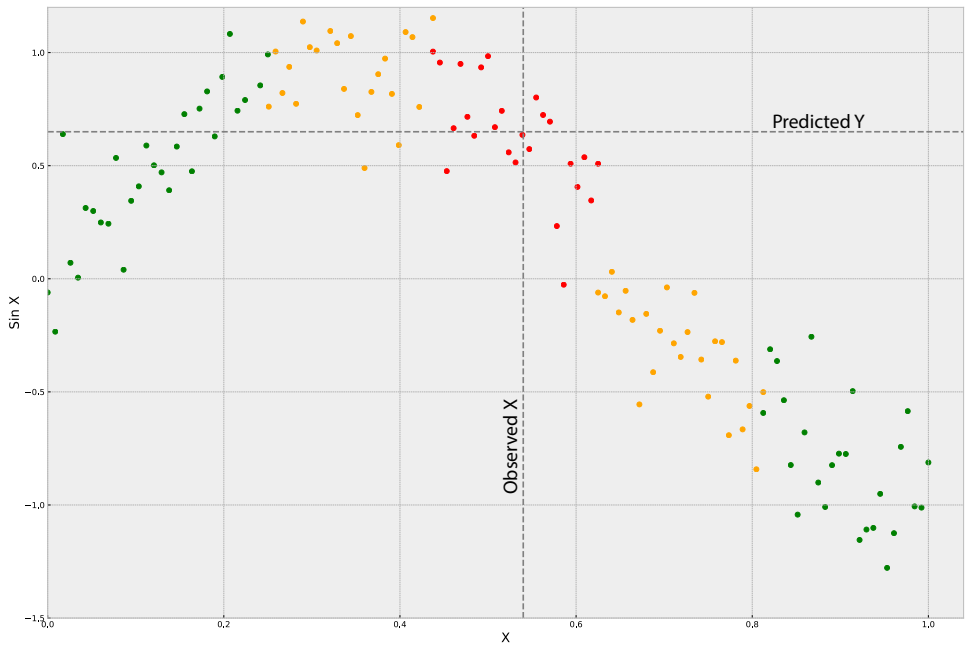
	Model search	Advantages	Disadvantages	Examples
Filter		Univariate: Fast Scalable Independent of the classifier	Ignores feature dependencies Ignores interaction with the classifier	Chi-square Euclidean distance t-test Information gain, Gain ratio [6]
		Multivariate: Models feature dependencies Independent of the classifier Better computational complexity than wrapper methods	Slower than univariate techniques Less scalable than univariate techniques Ignores interaction with the classifier	Correlation based feature selection (CFS) [45] Markov blanket filter (MBF) [62] Fast correlation based feature selection (FCBF) [136]
Wrapper		Deterministic: Simple Interacts with the classifier Models feature dependencies Less computationally intensive than randomized methods	Risk of over fitting More prone than randomized algorithms to getting stuck in a local optimum (greedy search) Classifier dependent selection	Sequential forward selection (SFS) [60] Sequential backward elimination (SBE) [60] Plus q take-away r [33] Beam search [106]
		Randomized: Less prone to local optima Interacts with the classifier Models feature dependencies	Computationally intensive Classifier dependent selection Higher risk of overfitting than deterministic algorithms	Simulated annealing Randomized hill climbing [110] Genetic algorithms [50] Estimation of distribution algorithms [52]
Embedded		Interacts with the classifier Better computational complexity than wrapper methods Models feature dependencies	Classifier dependent selection	Decision trees Weighted naive Bayes [28] Feature selection using the weight vector of SVM [44, 125]

Objective

In this research we investigated the capability of General Regression Neural Networks:

- to fully explore the input space, recognizing relevant, irrelevant and redundant features ("Isotropic" wrapper approach);
- to perform an internal weighting/ranking of the features ("Anisotropic" embedded/filter approach)

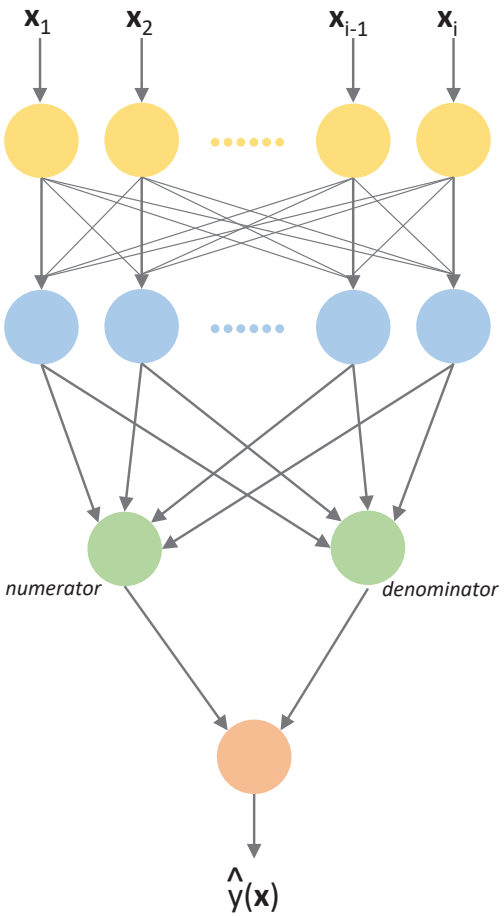
Nadaraya-Watson estimator



$$\hat{y}(\mathbf{x}) = \frac{\sum_{i=1}^{n} y_i \; exp\left(-D(\mathbf{x},\mathbf{x}_i)\right)}{\sum_{i=1}^{n} exp\left(-D(\mathbf{x},\mathbf{x}_i)\right)}$$

$$D(\mathbf{x},\mathbf{x}_i) = \sum_{j=1}^{p} \left(\frac{x_j - x_{ij}}{\sigma}\right)^2$$

General Regression Neural Network



$$\hat{y}(\mathbf{x}) = \frac{\sum_{i=1}^{n} y_i \; exp\left(-D(\mathbf{x},\mathbf{x}_i)\right)}{\sum_{i=1}^{n} exp\left(-D(\mathbf{x},\mathbf{x}_i)\right)}$$

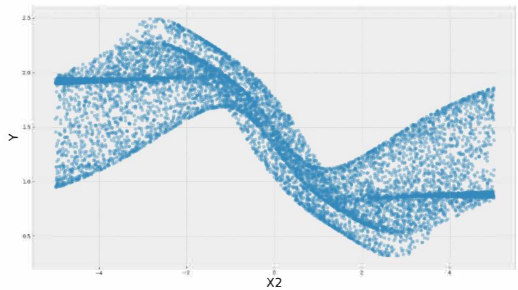
$$D(\mathbf{x},\mathbf{x}_i) = \sum_{j=1}^{p} \left(\frac{x_j - x_{ij}}{\sigma}\right)^2$$

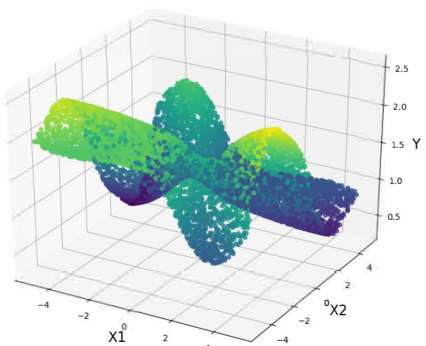
- "Isotropic": one bandwidth for all the features
- "Anisotropic": different bandwidth for each feature

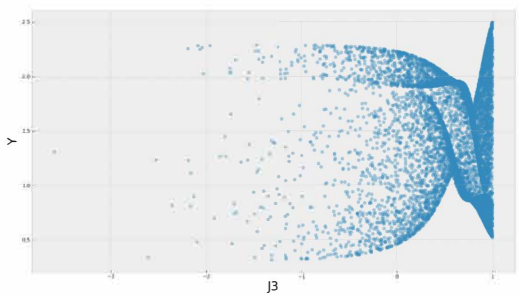
The butterfly dataset

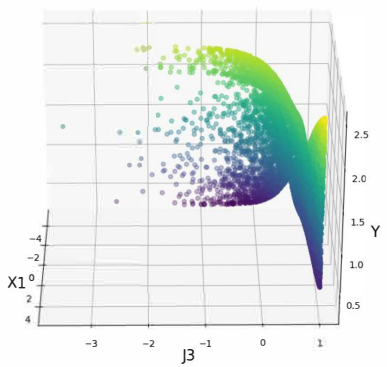
The *butterfly* dataset is constituted by one target variable (Y) and eight features, of which two are relevant (namely X_1 and X_2), three are redundant (J_3, J_4 and J_5) and three are irrelevant (I_6, I_7 and I_8).

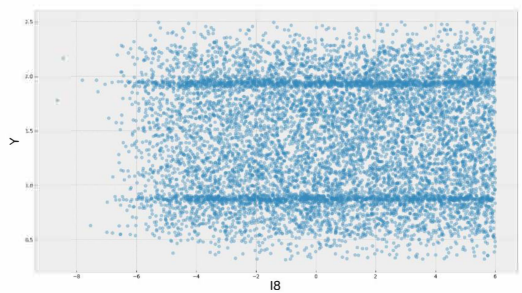
Relevant **Redundant** **Irrelevant**.

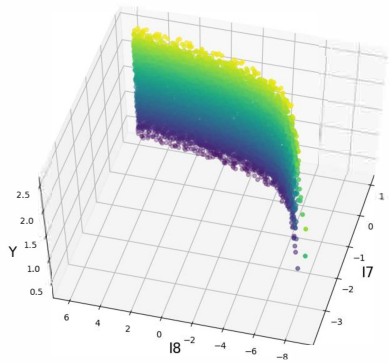












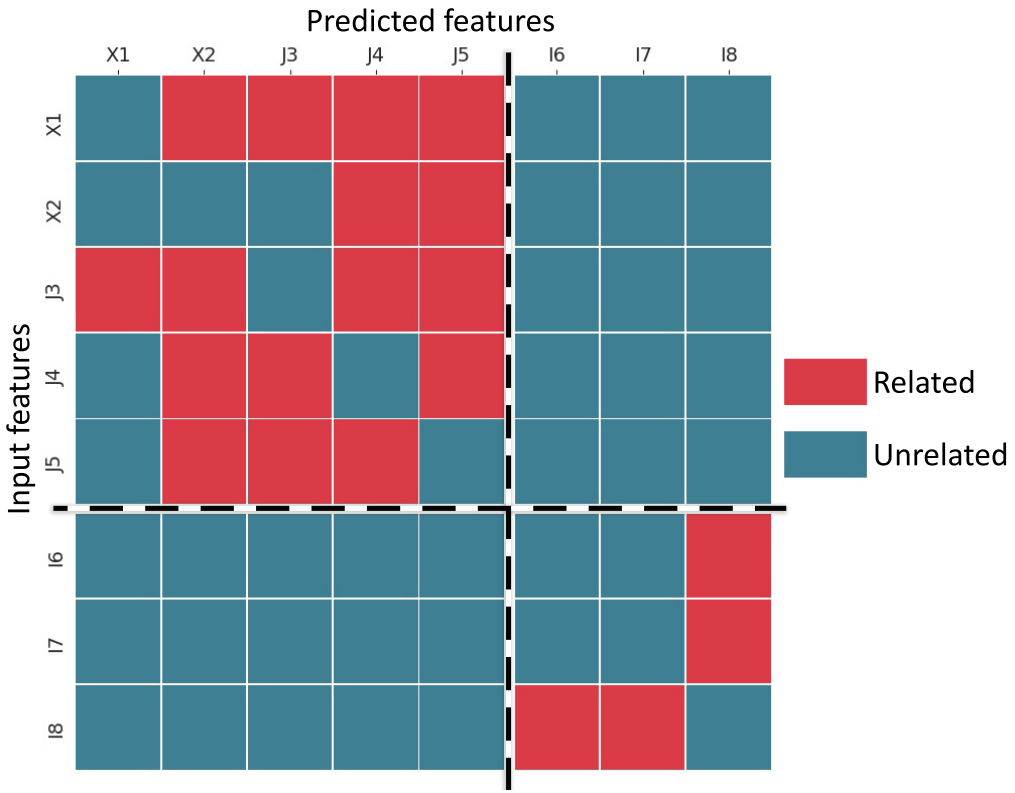
Isotropic Selector (IS)

We use one bandwidth σ for all the variables (features)

- Plug-in bandwidth $= 0.9\hat{\sigma}_j n^{\frac{-1}{(4+p)}}$
- Low training time!!!
- We can fastly perform an exhaustive search over the $2^p - 1$ possible combination of features to find the one minimizing the training MSE
- Limitation: not applicable in case studies with extremely large p

STEP 1: Analysis of dependencies in the input space

Relatidness: non-linear predictability of an input variable using the other features of the input space (without considering Y).



STEP 2: Feature selection

Relevant

Features in the subset minimizing the CV-MSE in an exhaustive search (or a forward-backward feature selection);

Redundant

Features **related** to the relevant ones, i.e. included in the subset minimizing the CV-MSE in an exhaustive search (or a forward-backward feature selection) when using as output the relevant features;

Irrelevant

Features which are neither relevant nor redundant.

Feature selection, *butterfly* dataset

% of noise	relevant	redundant	irrelevant
10%	(X_1, X_2)	(J_3, J_4, J_5)	(I_6, I_7, I_8)
20%	(X_1, X_2, J_4)	(J_3, J_4, J_5)	(I_6, I_7, I_8)
30%	(X_1, X_2, J_4)	(J_3, J_5)	(I_6, I_7, I_8)
40%	(X_1, X_2, J_4)	(J_3, J_5)	(I_6, I_7, I_8)
50%	(X_1, X_2, J_4)	(J_3, J_5)	(I_6, I_7, I_8)
75%	(X_1, X_2, J_4, J_5)	(J_3)	(I_6, I_7, I_8)
100%	(X_1, X_2, J_4, J_5)	(J_3, I_7)	(I_6, I_8)

Table: Result of the feature selection using IS on the butterfly dataset with **different percentages of noise injected in the input**

Anisotropic selector (AS)

In the *anisotropic* case, we consider a different bandwidth for each dimension (feature).

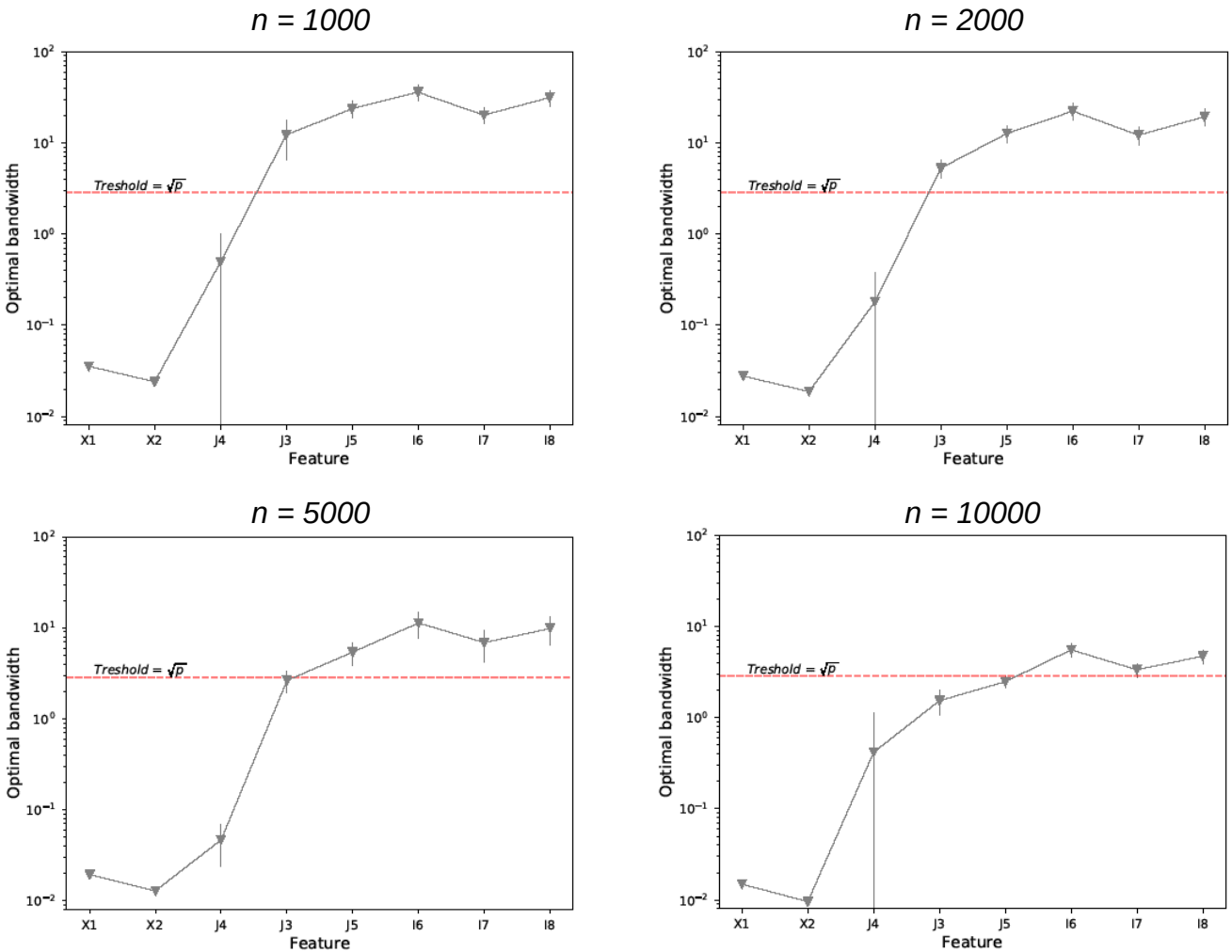
$$\hat{y}(\mathbf{x}) = \frac{\sum_{i=1}^{n} y_i \, exp\left(-D(\mathbf{x}, \mathbf{x}_i)\right)}{\sum_{i=1}^{n} exp\left(-D(\mathbf{x}, \mathbf{x}_i)\right)} \tag{1}$$

$$D(\mathbf{x}, \mathbf{x}_i) = \sum_{j=1}^{p} \left(\frac{x_j - x_{ij}}{\sigma_j} \right)^2 \tag{2}$$

Irrelevant

The j_{th} variable is irrelevant if σ_j is higher than a $\sqrt{p}$ (i.e. the maximum euclidean distance between two points in the hyper-cube defined by the Xp inputs)

Feature weighting, *butterfly* dataset



Feature shuffling, *butterfly* dataset

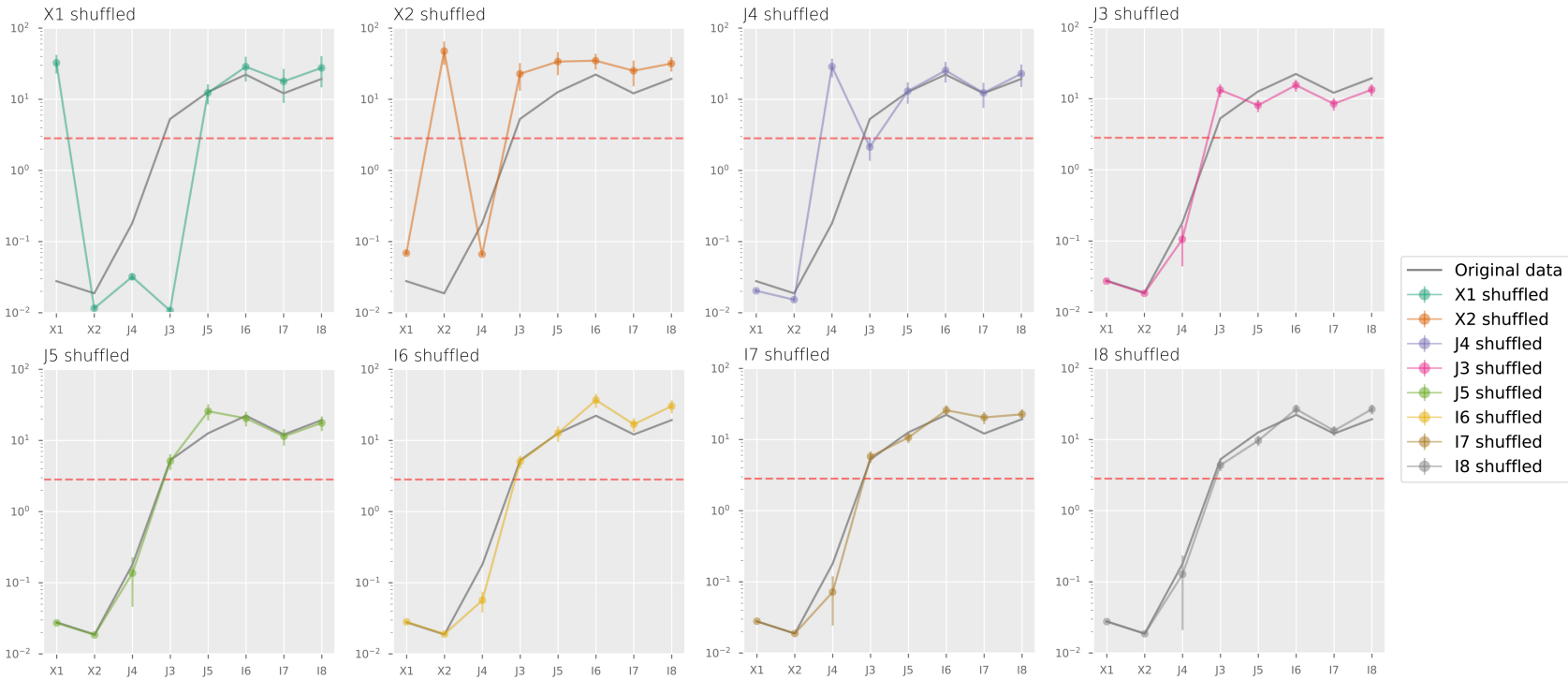


Figure: Mean and 95% confidence interval for the optimal bandwidth values after shuffling each feature on a butterfly dataset having $n = 2000$.

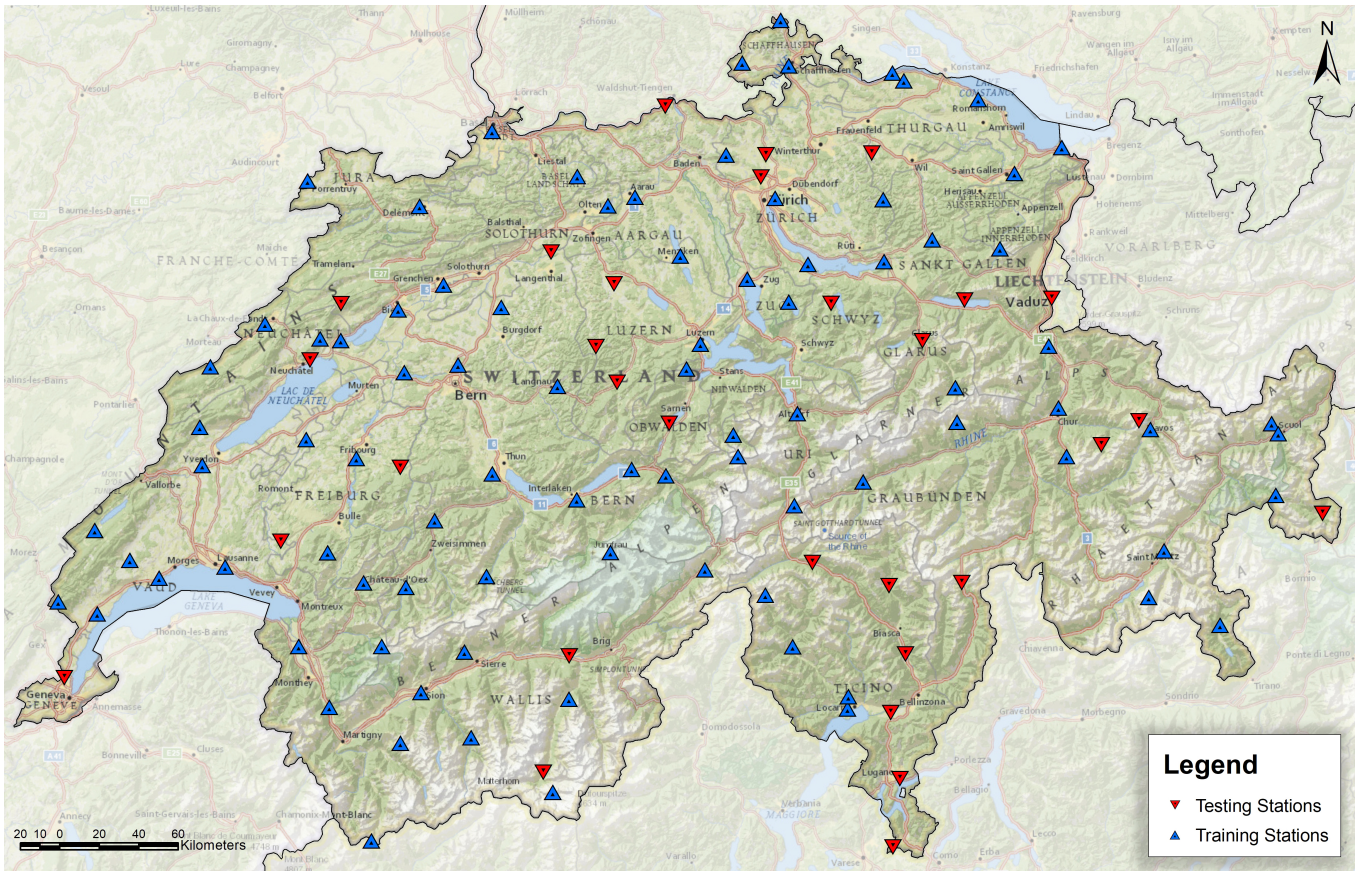
Spatial prediction of wind speed in Switzerland

Modelling 60 minutes frequency data from 118 stations in Switzerland from 2012 to 2013

- spatially-model the phenomena
- Feature space includes 13 spatial features
- Is FS part of the preprocessing or do we have to include it dinamicall in the modelling stage? (time-transferrability of the model)

The MeteoSwiss network

The 118 station were randomly splitted into training and testing

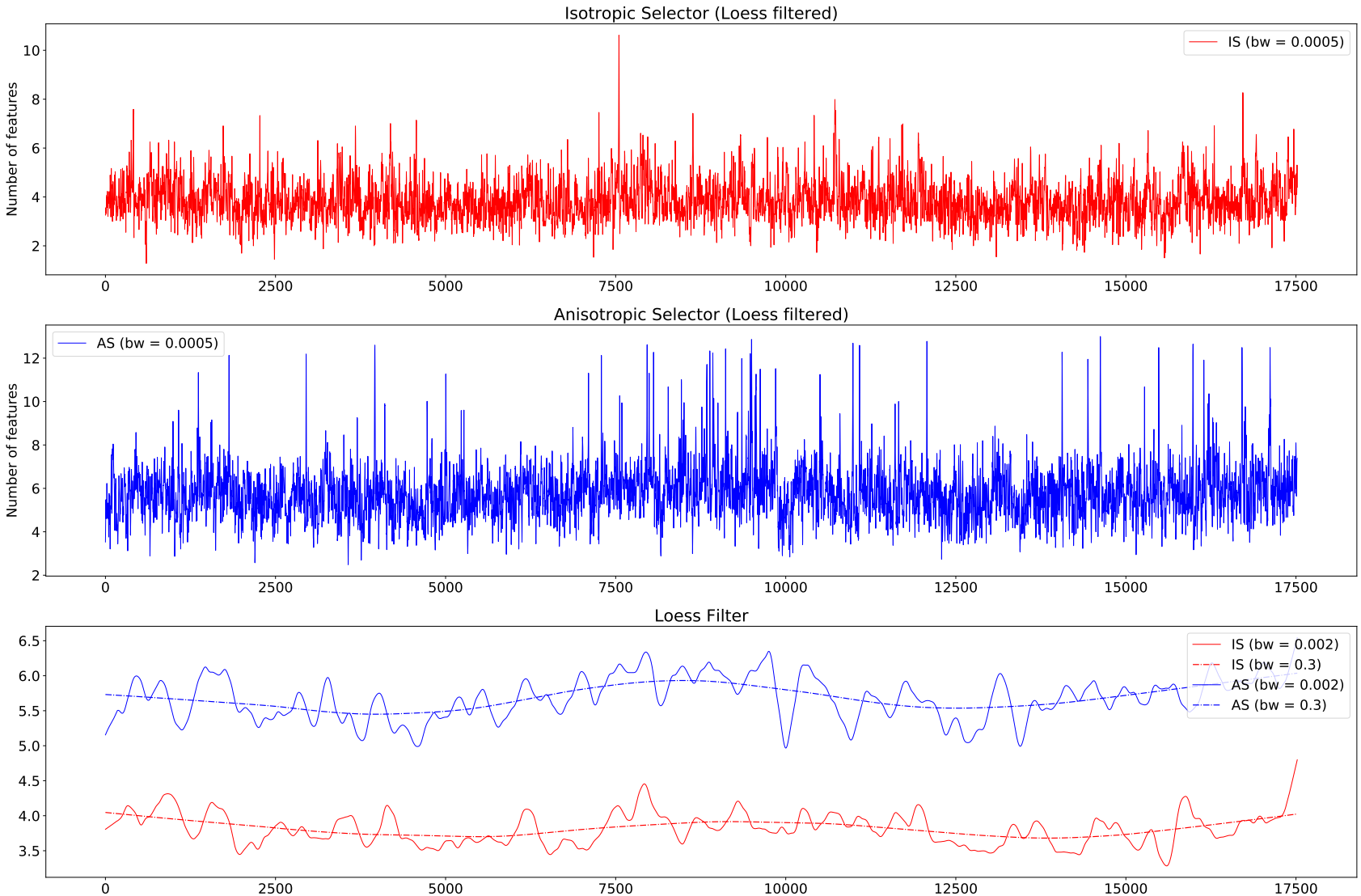


Spatial features

A 13-d input space has been designed including the geographical space (latitude, longitude and elevation) and features derived by applying filters and derivatives on the digital elevation model.

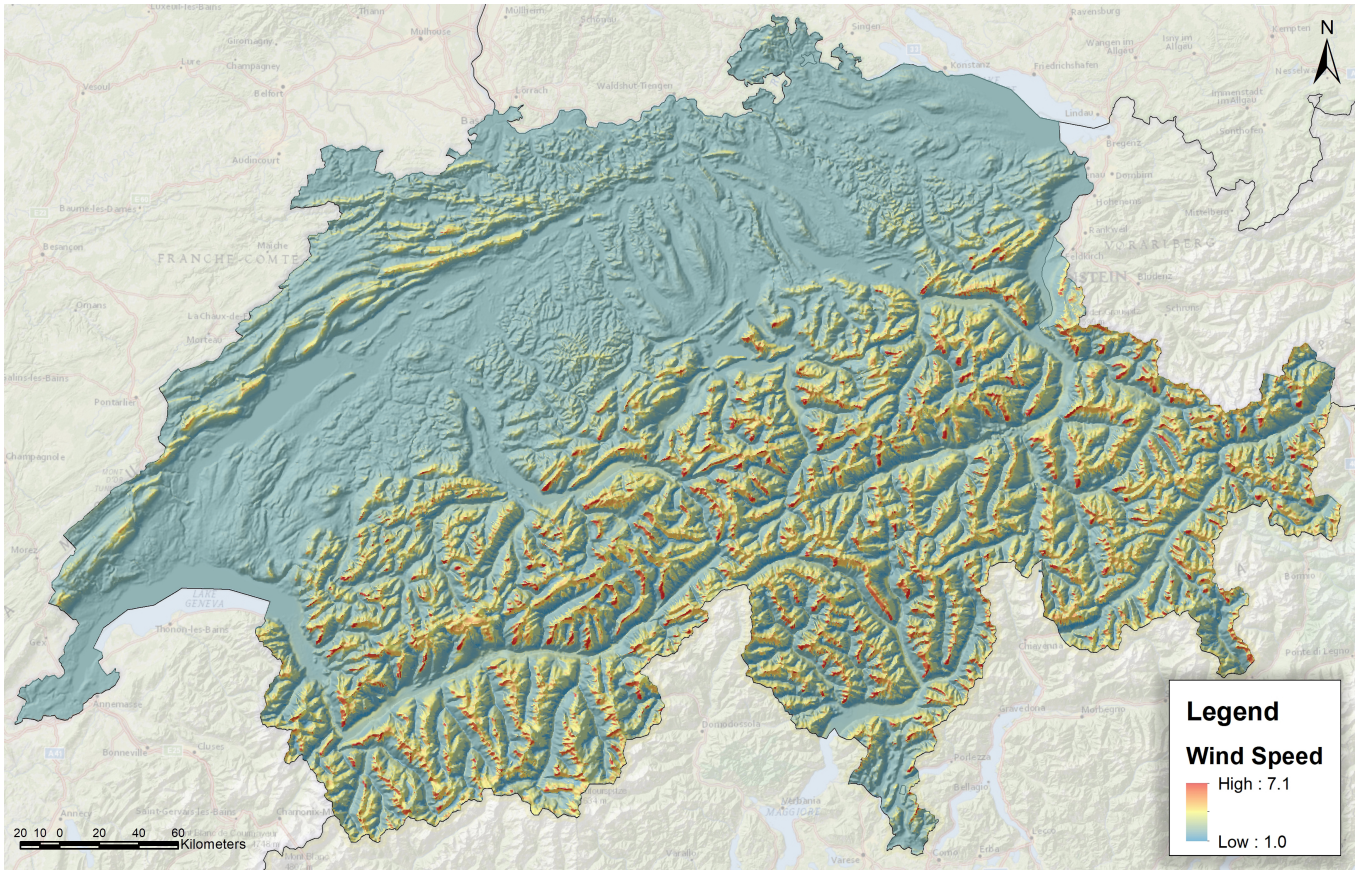
Feature	**Bandwidth**
Latitude	-
Longitude	-
Elevation	-
Difference of Gaussian (large scale)	$\sigma_1 = 3.75\ km, \sigma_2 = 5.55\ km$
Difference of Gaussian (medium scale)	$\sigma_1 = 1.75\ km, \sigma_2 = 2.25\ km$
Difference of Gaussian (small scale)	$\sigma_1 = 0.25\ km, \sigma_2 = 0.05\ km$
Slope (large scale)	$\sigma = 3.75\ km$
Slope (medium scale)	$\sigma = 1.75\ km$
Slope (small scale)	$\sigma = 0.20\ km$
Directional derivative E-W (medium scale)	$\sigma = 1.75\ km$
Directional derivative E-W (small scale)	$\sigma = 0.25\ km$
Directional derivative N-S (medium scale)	$\sigma = 1.75\ km$
Directional derivative N-S (small scale)	$\sigma = 0.25\ km$

Hourly data - Number of Selected Features



Spatial prediction (automatic mapping)

Wind speed prediction for April, 1 2012 12:00 using the best subset of features obtained with the Isotropic selector.



Conclusions

- The curse of dimensionality imposes to find new solution to reduce the dimensionality of our data
- We proposed two method based on GRNN to remove the non relevant variables from the input space (IS, AS)
- The application to wind speed showed how FS has to be intended as a dynamical stage in the modelling process

PyGRNN

The package *pyGRNN* has been implemented in Python and it is freely available.

- GitHub: https://github.com/federhub/pyGRNN
- Install in Python using *pip install pyGRNN*

Other dimensionality reduction tools

On the GeoKDD Lab webpage (https://wp.unil.ch/geokdd) you will find other resources for Dimensionality Reduction:

- **IDmining** - *Intrinsic Dimension for Data Mining*. Contains techniques for mining large and high-dimensional data sets by using the concept of Intrinsic Dimension. Author: Jean Golay
- **SFtools** - *Space Filling Based Tools for Data Mining*. Unsupervised dimensionality reduction tool to remove redundancy. Author: Mohamed Laib

SDS Meeting 2020

See you in Lausanne at the Spatial Data Science Meeting, from the 3rd to the 5th of June 2020!

- Info at https://wp.unil.ch/sds2020/
- Follow on Twitter @SDSMeeting2020

75 NRP Big Data National Research Programme
FNSNF Swiss National Science Foundation

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