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Local Machine Learning Models for Spatial Data Analysis

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Abstract. In this paper, we compare different machine learning algorithms applied to non stationary spatial data analysis. We show that models taking into account local variability of the data are better than models which are trained globally on the whole dataset. Two global models (Support Vector Regression and Multilayer Perceptrons) and two local models (a local version of Support Vector Regression and Mixture of Experts) were compared over the Spatial Interpolation Comparison 97 (SIC97) dataset, and the results are presented and compared to previous results obtained on the same dataset.

1 Introduction

During the last decade, machine learning algorithms, such as artificial neural networks, have been extensively used for a wide range of applications. They have been applied for classification, regression, and density estimation tasks (see [1] for a good overview). In fact, many fields of research using feature extraction or data prediction (and there are many) have been trying some machine learning models, with more or less success. Analysis of spatial data has been involving these methods as well, like in [10] and [4], but such ideas are not so much exploited for what concerns Geostatistical data.

One possible reason to this can be the "black box" aspect of most of these algorithms. Tuning them can be very difficult and without a clear methodology and some prior information about data, it can often lead to bad results. Another reason is that the tuning of most learning algorithms is partly based on theoretical machine learning arguments and rarely on some expertise on the problem to solve, and thus difficult to interpret. Therefore, it can appear unnecessary to use such complex methods when one have more simple but yet efficient one. However when the simple methods can no longer be applied due to the complexity of the data, these machine learning algorithms have to be considered in order to expect better results at the price of loosing some interpretability of the underlying models.

In this paper, we try to demonstrate the potential of machine learning algorithms, showing that a specific adaptation to the given problem of two basic learning methods, multilayer perceptron and support vector regression, can improve significantly their performances on a given dataset. One of these adaptations (mixture of experts) is a direct usage of an existing machine learning algorithm, and the other one (local support vector regression) is a modification of the training procedure of the original algorithm, using Geostatistical *a priori* knowledge, in a similar way than it has been done by De Bollivier *et al* for local multilayer perceptron[4].

In the following two sections, we introduce the methods compared in this paper, first the global methods (support vector regression and multilayer perceptron), and then the local methods (local support vector regression and mixture of experts). The next section is then devoted to the methodology we used in order to select the values of the hyper-parameters of all machine learning algorithms in order to avoid any bias. Finally, in the experimental section, we apply all these methods to the Spatial Interpolation Comparison 97 [6] dataset, and compare and comment the results.

2 Global Models

2.1 Support Vector Regression

Directly derived from Vapnik and Chervonenkis' *Statistical Learning Theory* [14], Support Vector Machines (SVM) for classification problems were developed during the beginning of the 90's (a good overview of SVMs can be found in [3]). Later, the algorithm was extended to deal with regression problems. This new algorithm was thus named Support Vector Regression (SVR) [13], and we present it here briefly.

For a given set of data $(\mathbf{x}_i, y_i)_{1 \le i \le l}$, $\mathbf{x} \in \mathbb{R}^n$ and $y \in \mathbb{R}$, the simplest linear SVR algorithm tries to find the function

$$f(\mathbf{x}) = w \cdot \mathbf{x} + b$$

minimizing the quadratic optimization problem

$$\frac{1}{2}\|w\|^2 + C \sum_{i=1}^{l} Q(y_i - f(\mathbf{x}_i))$$

where, in our case $Q(x) = max\{0, |x| - \epsilon\}$ corresponds to Vapnik's ϵ-insensitive loss function, which does not penalize errors less than $\epsilon \ge 0$ (cf. Figure 1). After some reformulation and taking into

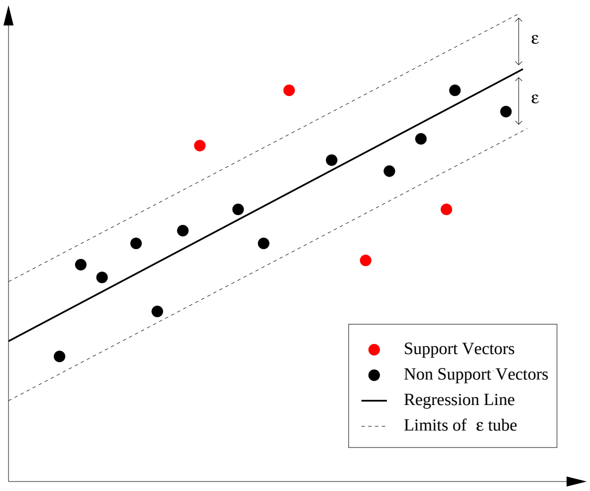


Figure 1: SVR linear regression with ϵ-insensitive loss function.

account the case of non-linear regression, the optimization problem is then transformed into the minimization of

$$\frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}(\alpha_i-\alpha_i^*)(\alpha_j-\alpha_j^*)k(\mathbf{x}_i,\mathbf{x}_j)+\epsilon\sum_{i=1}^{l}(\alpha_i+\alpha_i^*)-\sum_{i=1}^{l}y_i(\alpha_i-\alpha_i^*)$$

subject to

$$\sum_{i=1}^{l}(\alpha_i-\alpha_i^*)=0$$
$$0\le\alpha_i,\alpha_i^*\le C,\ \text{for } 1\le i\le l$$

where the α_i, α_i^* are Lagrange multipliers, solutions of the optimization problem, C is the *soft margin* parameter, weighting the influence of the loss function against the regularization term, and $k(\mathbf{x}_i, \mathbf{x}_j)$ is a *kernel function*, defining the feature space in which the optimal solution of the problem will be computed in order to handle non-linear problems. In our experiments, we used the Gaussian Radial Basis Function (RBF) kernel:

$$k(\mathbf{x}_1,\mathbf{x}_2)=\exp\left(-\frac{\|\mathbf{x}_1-\mathbf{x}_2\|^2}{2\sigma^2}\right).$$

To estimate a new point, we then use the following function f:

$$f(\mathbf{x})=\sum_{i=1}^{N}(\alpha_{s_i}-\alpha_{s_i}^*)k(\mathbf{x},\mathbf{x}_{s_i})+b$$

where the $s_i, 1 \le i \le N$ are the indices of the data points for which either α_{s_i} or $\alpha_{s_i}^*$ is non zero. Those points are called *support vectors* (red points in Figure 1).

2.2 Multilayer Perceptrons

A multilayer perceptron (MLP) is a particular architecture of artificial neural networks, composed of layers of non-linear but differentiable parametric functions. For instance, Figure 2 shows an MLP

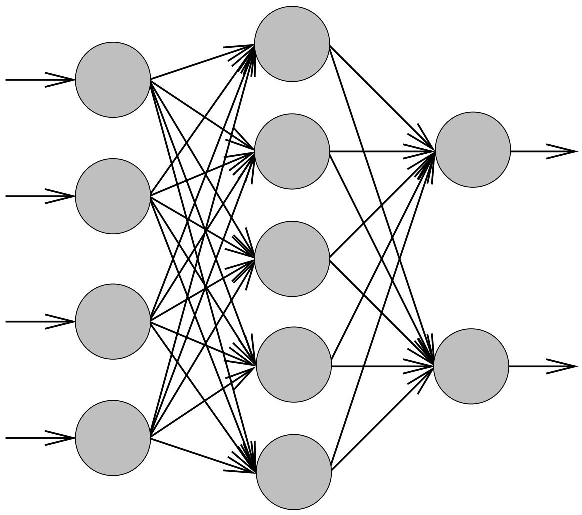


Figure 2: The architecture of an MLP.

with one input layer of size 4, one hidden layer of size 5 and one output layer of size 2. Alternatively, an MLP can be written mathematically as follows:

$$f(\mathbf{x};\theta) = b + \sum_{n=1}^{N} w_n \cdot \tanh\left(b_n + \sum_{m=1}^{M} x_m \cdot w_{nm}\right)$$

where the estimated output $f(\mathbf{x};\theta)$ is a function of the input vector $\mathbf{x}$ (indexed by its M values x_m), and the parameters $\{\theta : w_n, w_{nm}, b_n, b;\text{ with } n \in [1, N], m \in [1, M]\}$. This MLP is thus a weighted combination of N hyperbolic tangents of weighted combinations of the input vector. Given a criterion Q to minimize, such as the mean squared error,

$$Q = \sum_{i=1}^{l} (y_i - f(\mathbf{x}_i;\theta))^2$$

between the desired output y_i and the estimated output $f(\mathbf{x}_i;\theta)$, for a given training set of size l, one can minimize such criterion using a gradient descent algorithm [12]. This algorithm is based on the computation of the partial derivative $\frac{\partial Q}{\partial \theta}$ of the criterion Q with respect to all the parameters θ of $f(\mathbf{x};\theta)$. The gradient descent can then be performed using

$$\theta = \theta - \lambda \cdot \frac{\partial Q}{\partial \theta}$$

for each parameter θ where λ is the *learning rate*. It has been shown that given a number of hyperbolic tangents N sufficiently large, one can approximate any continuous function using such MLPs [8].

3 Local Models

As proposed by Bottou and Vapnik in [2], when the data is clearly non-evenly distributed, one can significantly improve the prediction results of machine learning algorithms by building multiple local models instead of one global model. In this section, we propose the use of two local methods, based respectively on SVRs and MLPs.

3.1 Local SVR

The proposed algorithm builds one SVR model for each point to be estimated, taking into account only a subset of the training points. This subset is chosen on the basis of the Euclidean distance between the testing point and the training point in the input space. For each testing point, a new SVR model is thus learned using only the training points lying inside a user defined radius which center is the current testing point.

The radius can be chosen in relation to the *a priori* spatial correlation of the data, or like any other hyper-parameters, i.e. by cross-validation (see section 4 for an introduction to cross-validation). It is also possible to use an anisotropic neighborhood, for example an ellipsoïd, instead of a circle. With such a point selection, one can "force" the local model to adapt itself to an anisotropic phenomenon.

A problem related to local SVR estimation (besides the computational time needed to create all these local models) concerns the number of points in the subset. If the selected radius is too small, it might happen that some testing points will have a very small number of training points in their subset (or even none). Theoretically, the SVR algorithm can work even with only two training points (with input vectors in two dimensions). But due to numerical stability of the optimization, it is better not to estimate any SVR model with less than four training points. Testing points in this situation can thus be estimated by simple mean value or inverse distance, which would not be very different from what SVR would have predicted on such a small number of point.

On the contrary, if the research radius is large, one might have a very large number of training points, which can lead to long training time, considering the fact that we are computing one model for each testing point! Thus, in order to speed up the procedure, one might consider to limit the number of training points taken into consideration. It is also important to note that testing points very close to each other will probably have the same neighbors in the training set, and thus, only one model should be necessary to predict those testing points.

3.2 Mixture of Experts

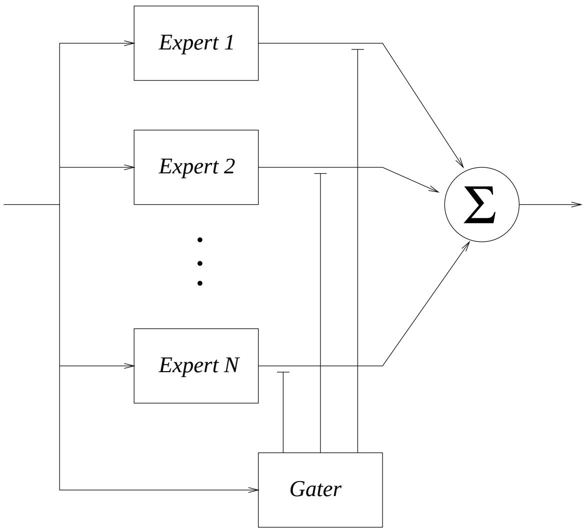


Figure 3: The architecture of a mixture of experts.

A mixture of experts [9] is a very simple model that embodies the divide-and-conquer principle: instead of trying to fit a unique model for a whole training set, one supposes that dividing the training set into many smaller training sets could simplify the problem. The idea of a mixture of experts is then to simultaneously (a) learn a *soft* division of the training set into different parts[1] and (b) learn a different model on each part. As shown if Figure 3, in its simplest form, a mixture of experts is thus composed of N modules, each receiving the same inputs, and each trying to output the desired target. An additional module, the *gater*, also receives the same input but has N outputs which corresponds to the probability of each module to give the correct target. It thus computes a soft partition of the input space. More formally, for each input/output point $(\mathbf{x}_i, y_i)$, each model m_n is computing $E(y_i|\mathbf{x}_i, m_n)$ the expectation of the output y_i given the input $\mathbf{x}_i$, and the gater is computing $P(m_n|\mathbf{x}_i)$ the probability of model m_n given the input $\mathbf{x}_i$. The overall output of the mixture of experts is then

$$E(y_i|\mathbf{x}_i) = \sum_{n=1}^{N} P(m_n|\mathbf{x}_i) E(y_i|\mathbf{x}_i, m_n)$$

with the constraint that

$$\sum_{n=1}^{N} P(m_n|\mathbf{x}_i) = 1.$$

In the particular case where the gater and the models are represented by differentiable parametric functions such as multilayer perceptrons[2], the whole system can be optimized jointly by minimizing an overall criterion Q such as the mean squared error over the whole training set. For parameters θ of a given model m_n, the derivative of the criterion with respect to the parameters is as follows

$$\frac{\partial Q}{\partial \theta} = \sum_{i=1}^{l} \frac{\partial Q}{\partial E(y_i|\mathbf{x}_i)} \frac{\partial E(y_i|\mathbf{x}_i)}{\partial E(y_i|\mathbf{x}_i, m_n; \theta)} \frac{\partial E(y_i|\mathbf{x}_i, m_n; \theta)}{\partial \theta}$$

and for parameters θ of the gater, the derivative is as follows

$$\frac{\partial Q}{\partial \theta} = \sum_{i=1}^{l} \frac{\partial Q}{\partial E(y_i|\mathbf{x}_i)} \sum_{n=1}^{N} \frac{\partial E(y_i|\mathbf{x}_i)}{\partial P(m_n|\mathbf{x}_i; \theta)} \frac{\partial P(m_n|\mathbf{x}_i; \theta)}{\partial \theta}.$$

Finally, it is important to note that one does not have to decide the partition of the training set but still has to decide the number of such partitions. This can be done using for instance a cross-validation technique, as described in section 4 on Model Selection.

3.3 Local Models and Geostatistics

As Geostatistical data are often influenced by various local phenomena, the idea of using local models applied to Geostatistical problems was also developed for classical Geostatistical interpolation methods, like ordinary kriging [7] as well as with MLPs [4]. In the latter however, the authors do not use mixture of experts but instead they propose to use MLPs trained using local data, in a similar way as we proposed to use local SVRs.

4 Model Selection

Most of the models proposed in the machine learning literature, and all the models proposed in this paper, have some *hyper-parameters* that need to be selected prior to learning. *Hyper-parameters* are parameters of the algorithm that are defined by the user and which influence the training procedure. For instance, for an iterative algorithm, it could be the number of iterations; for a multilayer perceptron, it could be the number of hidden units; for a support vector machine, it could be a parameter

[1] As it will be seen with the equations, instead of attributing an example to one and only one model, each model will see every examples but with a different weight for each example.

[2] Note that in order for the gater to output probabilities, some special output function should be used to ensure the necessary constraints, such as the well-known *softmax* function $y_i = \frac{e^{x_i}}{\sum_{j=1}^{N} e^{x_j}}$.

related to the chosen kernel; in fact, most of the models usually have more than one hyper-parameter. In order to select them appropriately, some kind of *hyper-learning* method is needed.

The method depends on the size of the dataset. When it is large enough (usually more than a few thousand examples), a simple method works as follows:

- Randomly divide the dataset into two parts, a *training set* and a *validation* set (the validation set is usually smaller than the training set, depending on the total size of the dataset).
- For each value of the hyper-parameter (if there is more than one hyper-parameter then, for each set of values of the hyper-parameters), train a model on the *training set* and compute the performance of the trained model on the *validation set*.
- Select the value of the hyper-parameter that produced the model that gave the best performance on the *validation set* and train the corresponding model with the whole dataset.

The main idea behind this method is that the hyper-parameters have to be chosen with data that were not used for training in order to avoid any bias. However, when the size of the dataset is too small, which is often the case in Geostatistical problems, this simple method becomes too noisy and depends strongly on the arbitrary division between the training and the validation sets. An extension of this method, called *cross-validation*, and which have many variants, should then be used. For the current study, we used the *K-fold cross-validation* method:

- For each value of the hyper-parameter (if there is more than one hyper-parameter then, for each set of values of the hyper-parameters), estimate the *generalization* performance of the corresponding model as follows:
  - Randomly divide the dataset into K partitions of approximately the same size.
  - For each partition, train a model using the data from the $K-1$ other partitions and compute the generalization performance of all the examples of this partition.
  - Add all generalization performances to compute the overall generalization performance of the model with the current value of the hyper-parameter.
- Select the value of the hyper-parameter that produced the model that gave the best generalization performance and train the corresponding model with the whole dataset.

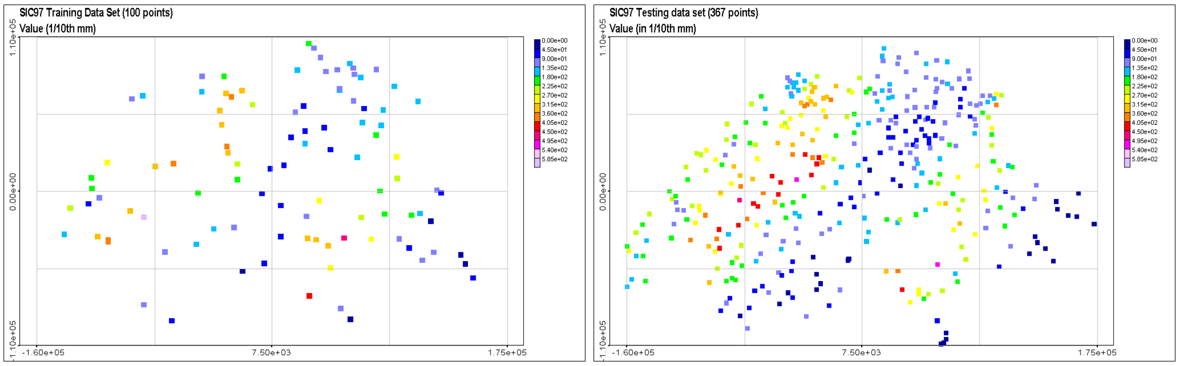
Note that these methods do not give a good estimate of the performance of the selected model on new data since all the examples have been used to select the model. When one wants also to estimate the generalization performance of the selected model, one needs to do two embedded *cross-validations*: one to select the right model and one to estimate its performance. In the current study, we did not estimate the generalization performance since the goal was to select a model and then give predictions on a separate dataset.

5 Case Study

5.1 Dataset

The dataset we used to compare local and global machine learning methods is the same as the one used in the Spatial Interpolation Comparison 97 (SIC97) [6]. It consists in 467 daily rainfall measurements made in Switzerland, splited into a training set of 100 points and a testing set of 367 points (Figure 4). Given the training set and a digital elevation model, SIC97 participants had to predict rainfall at the 367 locations of the testing set.

The SIC97 dataset is characterized by the small amount of training data and by a second order non-stationarity, which means that correlation between data values is not independent from data position, which is a sign of local phenomena. Another interesting challenge in the use of such a dataset is



(a) Training set

(b) Testing set

Figure 4: SIC97 training and testing datasets. The training set consists in 100 rainfall measurements in 1/10th of millimeters. The testing set consist in 367 measurement locations where rainfall must be predicted. The true values in 1/10th of millimeters are presented here.

that the training set distribution is slightly different from the whole dataset, information which was provided only *a posteriori* to the participants of the competition. Finally, a lot of contributions exists [6], from which only a few were based on machine learning algorithms. It is thus a good benchmark to compare methods.

5.2 Experimental Setup

In all experiments, only X and Y coordinates were used as input information. Experiments using also altitude did not improve significantly the results of the first model tried (the global SVR), and so, for a better comparison, it has not been used for the other models (but it might be done in a close future).

The choice of the hyper-parameters was done by K-fold cross-validation on the training data, inside a user defined set of hyper-parameters. Such an approach can become very time consuming when the number of hyper-parameters is high. It is therefore necessary to restrict the range in which these values should be selected.

5.2.1 Global SVR

The kernel parameter σ, which is the standard deviation of a Gaussian function, is directly related to the local variability of the data: the more the data is locally variable, the smaller it should be. In practice, it is of no use to compute a model with a value of σ greater than half the maximum distance between our data points: choosing such a high value would imply a very low variability and thus no significant improvement would rise from increasing the σ value. Following the same idea, σ cannot be smaller than half the smallest distance between the training points: this would imply a variability so high that no prediction would be possible as data points would be too far from each other (with respect to the Gaussian) to extract any correlation information.

The precision parameter ϵ has also an upper bound. It should not reach the difference between the highest and the smallest output values of the training set. If so, there would be no data points to compute the model, as they would all be considered as "acceptable mistakes". By the way, this upper bound is far too high in many cases. In [11], ϵ value is said to be upper-bounded by the value of the local variability of the data, the so called "nugget level" of the semi-variogram[3]. In SIC97 data, the

[3]The nugget level of a dataset corresponds to the value which the semi-variogram curve would have if one would

nugget effect is almost zero, so the optimal ϵ value should be very small with respect to data value, and a range from 0 to 50 was thus chosen.

The soft margin parameter C is much more difficult to limit. It is related to the confidence we have in our data: the highest it is, the more we believe in the training data. This hyper-parameter is unlimited, so usually, one gives it various powers of 10 in order to find the optimal one, but it might not be the most efficient method.

5.2.2 Local SVR

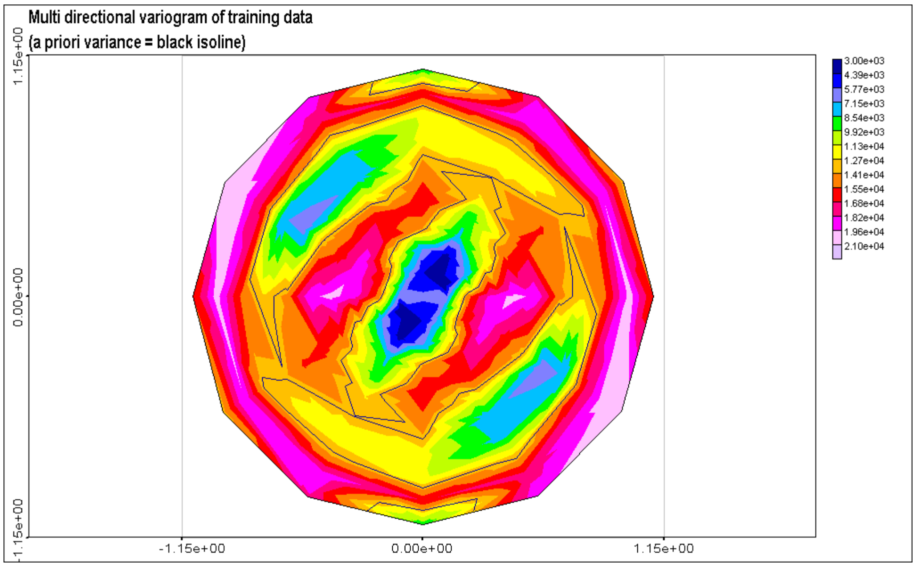


Figure 5: Multi-directional variogram of training dataset. The anisotropy of spatial correlation is clearly visible and can be used to improve the efficiency of prediction models.

For the local SVR, one has to define the search neighborhood, in addition to the other SVR hyper-parameters. This neighborhood was chosen with respect to the range and the anisotropy given by the semi-variogram of the whole training set (Figure 5). Of course, it might looks strange to use global parameters to compute local models. But due to the small number of data available, a computation of local semi-variograms would have been noisy and thus irrelevant. Moreover, a local adjustment of the anisotropic parameter would have been far too expensive in terms of computation time. Thus, the most important to extract the local correlation is to focus mainly on the first lags of the variogram, which are more likely to be related to the local correlation.

5.2.3 MLP

For the multilayer perceptrons, we had to select the number of hidden units (N), the number of learning iterations, and the value of the learning rate (λ). In fact, instead of using a simple gradient descent method, we used a conjugate gradient method, which takes into account second order information and do not need to select a learning rate λ. All these hyper-parameters are related to the *capacity* of the learning system: the more examples one have, the higher the values of the hyper-parameters could be, but their optimal value are problem dependent and can only be chosen by cross-validation. Some simple rule of thumb still exists, such as the fact that the number of parameters (weights and

interpolate it to a distance of 0. This is a quite subjective value as it is impossible to calculate it precisely. It represents the local variability of the data or measurement noise, also called "nugget effect".

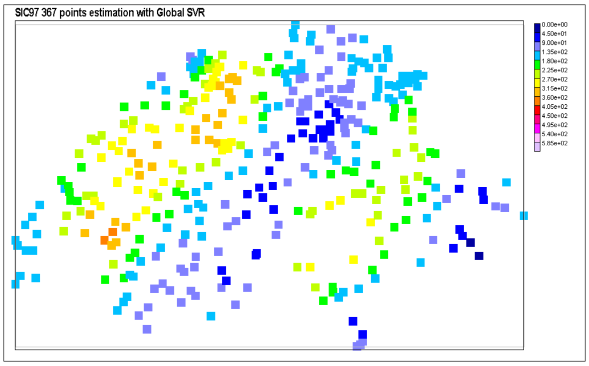
bias), which is related to the number of hidden units, is usually smaller than the number of training examples. But these rules of thumb should be used carefully, only to give an idea on the range of the values to select with cross-validation. The number of hidden units was thus chosen in a range from 5 to 40 and the number of iterations was chosen in a range from 100 to 1000.

5.2.4 Mixture of Experts

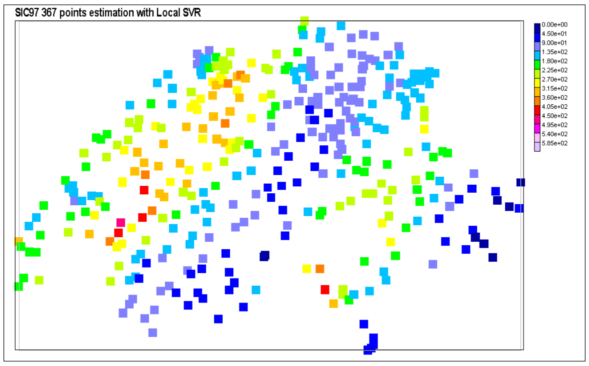
For the mixture of experts, we had to decide the number of experts and how to represent the experts and the gater. We decided to put most of the *capacity* into the gater so we represented it by an MLP, with various number of hidden units (from 5 to 40). The experts were then represented by simple linear models (weighted combinations of the inputs). The number of experts is not easy to select. It should reflect the non-stationarity of the data, but it should also take into account the total number of examples in the training set. Therefore, we chose it in a range from 2 to 12. Finally, the number of iterations was chosen in the same manner as for the MLP experiments.

5.3 Results

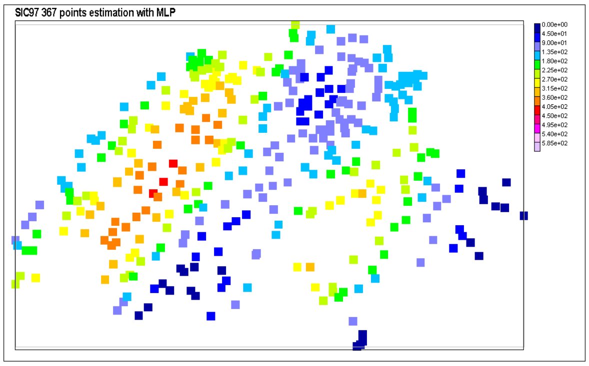
5.3.1 Visual Results



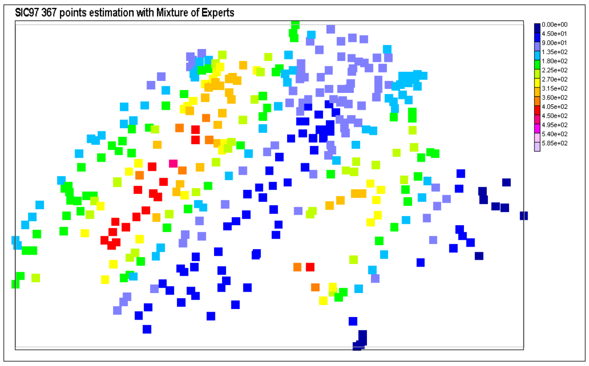
(a) Global SVR predictions



(b) Local SVR predictions



(c) MLP predictions

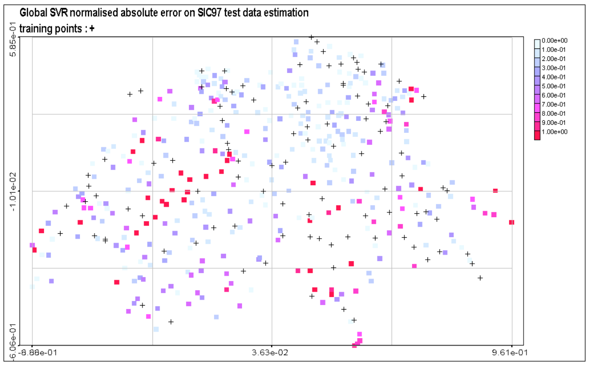


(d) Mixture of experts predictions

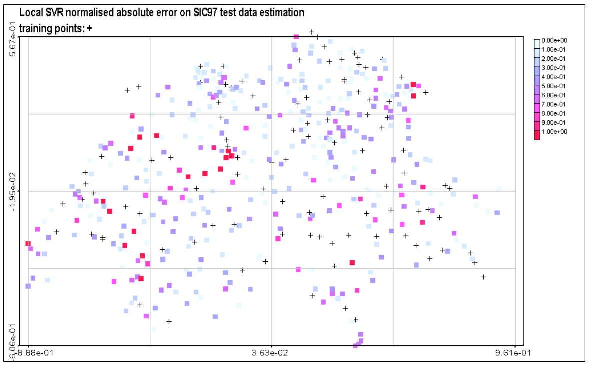
Figure 6: Estimations of SIC97 testing data with various machine learning models. The color scale is the same for all pictures and corresponds to the one of Figure 4.

Figure 6 is a visual comparison of SIC97 testing dataset predictions. Each of the four machine learning models studied is represented here.

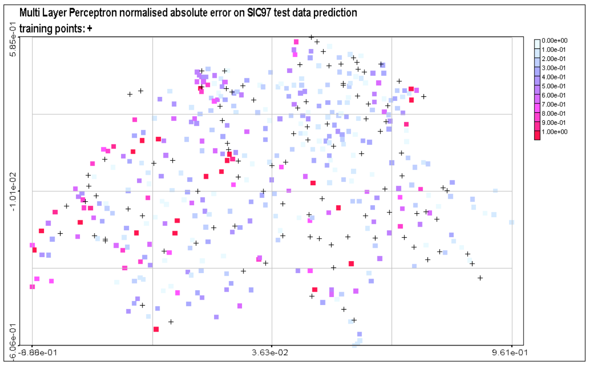
All the models did reproduce the large anisotropy of the SIC97 dataset, and the general predictions are quite close to the original data, with a large band of low precipitation from South-West to North-East, surrounded by two medium-to-high precipitation areas. The most visible difference between each model concerns the estimation of the extreme values. The global SVR failed in this task: the main tendencies are recovered, but the final result seems to be too smooth. The local SVR performs better in predicting high values and some very local phenomenon (like the "hot spot" in the West), but a large band of high rainfall is under-estimated. The MLP seems to perform better in the prediction of this high values band, but the North-West frontier is underestimated, as well as the hot spot detected by the local SVR. For the mixture of experts, the whole high precipitation region is predicted with a very good efficiency, and despite some difficulties in the North-West frontier, the general results seems to be the best of all four.



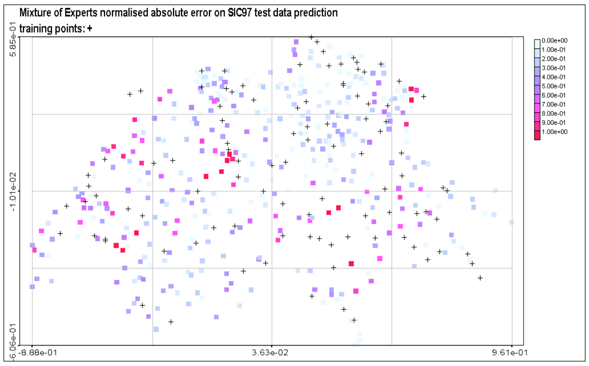
(a) Global SVR errors



(b) Local SVR errors



(c) MLP errors



(d) Mixture of experts errors

Figure 7: Normalized Absolute error of SIC97 testing data predictions. The normalized absolute error corresponds to the absolute error made by the predicting model at each location, divided by standard deviation of the whole SIC97 dataset (train + test). The position of the training points is represented by crosses.

A better overview of all this appears in Figure 7, which presents the normalized absolute prediction error made by each model. A first overview shows that the two global models are overall making higher errors than the two local models. Especially, the global SVR seems to fail in all extreme value predictions, while the MLP gives poor predictions in the North-West border. The local SVR and the mixture of experts are both significantly improving the performance of their global counterpart.

5.3.2 Spatial Correlation

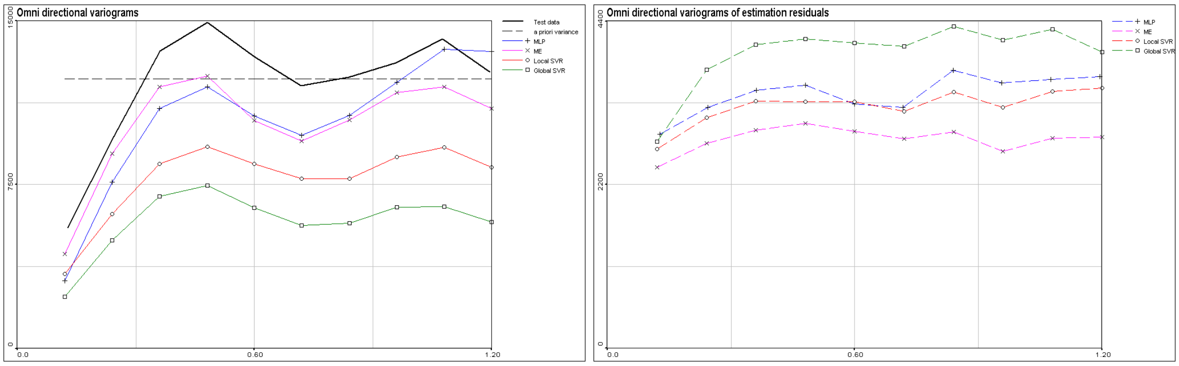


Figure 8: Omni-directional semi-variograms of SIC97 testing data estimations and residuals. The left figure shows the variograms from the four estimations, compared to the “true” one and to the *a priori* variance of the testing data. The right figure shows the variograms of the residuals of the four predictions, confronted to each other, in order to compare the remaining correlation inside error maps.

In Figure 8, one can compare the omni-directional semi-variogram of the original testing data to the ones obtained by the machine learning model estimations. It is interesting to notice that every four models managed to reproduce the general spatial correlation quite well over a large distance (the MLP is a bit worse at very large distance, but this is not really important). However, the global SVR estimation is very smooth, as the reduction of variance attests. This aspect of smoothing is also present for the local SVR, but the improvement with respect to the global SVR is quite significant. The MLP and the mixture of experts outperform both, reproducing almost exactly the rise of the short range correlation.

The variography of estimation residuals gives also some information about the feature extraction quality of each models for the SIC97 data. Thus, one can notice that the global SVR did not manage to extract all information, as residuals appears to be strongly correlated. But even if the remaining correlation is not as high, it exists also for the other methods, showing that some improvement is still theoretically possible. It is finally interesting to see that local models have improved the feature extraction capabilities of the global ones.

5.3.3 Numerical Results

Table 1 presents the numerical results of global and local model predictions of SIC97 testing dataset. In addition to root mean square error (RMSE) and mean absolute error (MAE), comparisons to the real SIC97 testing data statistics is also presented. The last part of the table summarizes the results of SIC97 as presented in [5]. “SIC97 best” and “SIC97 worst” gives the corresponding results, in terms of absolute deviation to the real value, found by the submitted models for this specific table section (i.e. the best RMSE and the best MAE do not correspond to the same model). “SIC97 median” gives the interval inside which the statistics of the best 50% of the submitted models are.

The numerical results give some complementary details compared to the pictures. First of all, we have a clear confirmation that, in terms of RMSE and MAE, local machine learning models perform better on SIC97 data than global ones. In addition, they are also able to reproduce quite efficiently

	RMSE	MAE	MIN	MEDIAN	MAX	MEAN	STDEV
SIC97 true	N.A.	N.A.	0	162	517	185	111
MLP	59	45.8	8.9	186.9	380.6	188.2	96.5
SVR	63.4	45.9	37.5	165.6	369.6	184	77.1
ME	53.2	38.6	0	165.3	453.8	182.5	101.7
Local SVR	57.1	41.9	0	163	472.7	182	88.8
SIC97 best	53.1	32	0	162	514	185	111
SIC97 median	63	44	[-15.5;15.5]	[154;170]	[462.5;571.5]	[181;189]	[99;123]
SIC97 worst	99	70.6	-413	191	788	159	139.5

Table 1: Comparison of multiple models over SIC97 dataset. The models compared were multilayer perceptrons (MLP), Support Vector Regression (SVR), mixture of experts (ME), and local SVR. They were compared to the best, median and worst results for the SIC97 competition. Results are given in terms of root mean squared errors (RMSE), mean absolute error (MAE), as well as some statistics such as the minimum predicted value (MIN), the median (MEDIAN), the maximum (MAX), the mean (MEAN) and the standard deviation (STDEV).

the general statistics of the data, which can be interpreted as a good estimation of the probability density of the dataset. This second aspect is particularly true for the local SVR. Compared to the MLP in terms of RMSE, these models are not significantly different[4], but when looking at general statistics, the local SVR is always better than the MLP, except for standard deviation conservation, as already shown in Figure 8.

Comparing now the results of the models to the general results from SIC97 contributions, one can notice first that all the machine learning algorithms presented here are at least as good as 50% of the methods published in 1998. Notice also that global models are worse to predict high extreme values (MAX < 462.5), and that SVR models have some difficulties to recover the variability of the data (STDEV < 99). Finally, the mixture of expert results appear to be one of the best published in terms of RMSE.

5.3.4 Conclusion on SIC97 Experiments

SIC97 benchmark, due to its complexity, has risen some drawbacks of global machine learning algorithms for Geostatistical data. While these methods were able to be almost as good as other regression techniques, they were less efficient than most model based approaches, like ordinary kriging. Various explanations can be formulated to explain this, but we can summarize them into the problem of quantity of information. As they are model free, learning algorithms are very sensitive to "bad" datasets. If the dataset is small and/or noisy, its probability distribution can be very far from the true probability distribution of the phenomenon. And without *a priori* knowledge, it becomes impossible to a learning algorithm to solve such problem efficiently. When used by experimented users, model based methods are often less sensitive to data representativity because the model becomes user's prior information about the phenomenon.

To limit these problems, we have chosen to build models focusing on local phenomena. In the case of the local SVR, we used some specific knowledge we had on data (such as spatial correlation and anisotropy) to artificially specialize the algorithm. Results are good as the improvement on all criteria is significant, with respect to the global SVR approach. The mixture of experts do not use more *a priori* knowledge than the underlying idea that one should focus on some local phenomena. And it is keeping some global information as it is building various global models locally weighted. As a consequence, it is able to extract phenomena to a larger scale than the local SVR (which is limited

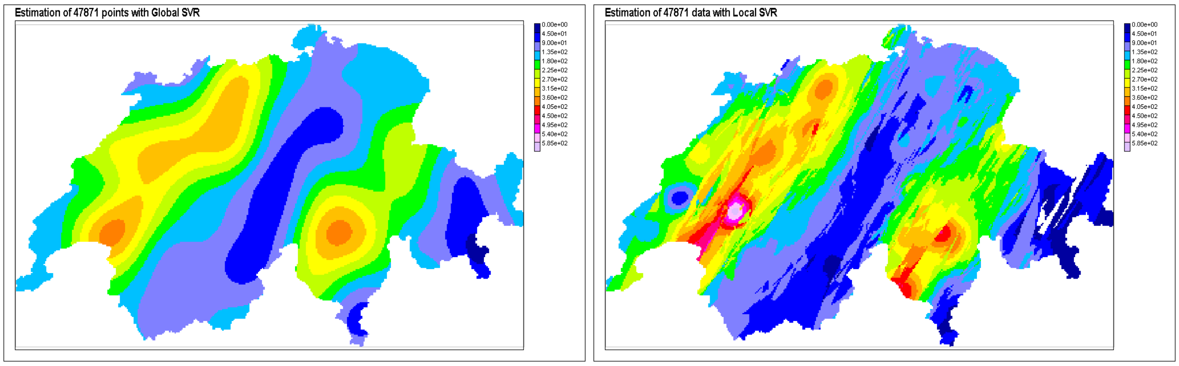
[4]However, the local SVR is better in MAE; this difference is probably related to the optimization criterion of each method.

by its search neighborhood), with thus a better prediction ratio, but generates a smoother structure (although more variable globally).

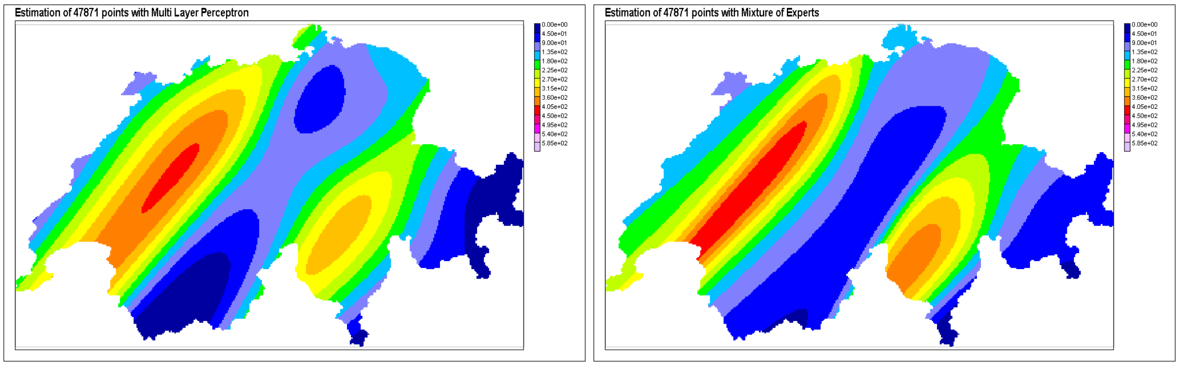
5.4 Beyond SIC97

Beyond the quantitative results of the Spatial Interpolation Comparison, it is interesting also to build some “precise” map of prediction of our models. Of course, it will be impossible then, to say quantitatively whether a model is better than another. But sometimes, a visual result is emphasizing some interesting details otherwise unseen by plain general statistical information, which is only a summary of a phenomenon.

5.4.1 Prediction on a Dense Grid



(a) Global SVR predictions (b) Local SVR predictions



(c) MLP predictions (d) Mixture of experts predictions

Figure 9: Prediction of a dense grid of 47871 points using the four models used for SIC97 data estimation. Color scale is similar to the one used for SIC97 estimation maps.

Figure 9 shows the prediction of the models on a dense grid of 47871 points. The difference between models predictions are impressive. First of all, one notices immediately the big difference between the global SVR, the MLP and the mixture of experts maps compared to the local SVR one. While the formers have a very regular and smooth behavior, the latter is very sharp and complex. This behavior is a direct consequence of the local modeling of the local SVR method. While the global SVR and the

MLP are using one model for all predictions, and the mixture of experts is using a linear combination of a small number of them, the local SVR approach is using, in the present estimation, around 2000 models applied to very specific regions. The absence of overlapping between the models explains the numerous discontinuity in the picture, and the local spots are a result of the different optimal hyper-parameters found during the training procedure. Finally, the strong anisotropy imposed to the training procedure is very easy to identify. Too easy to be realistic, in fact.

Even less realistic for a rainfall map are the other three pictures. The global SVR one has the characteristic round-shape behavior of radial basis functions. These shapes are very different from the one given by the MLP, closer to an ellipsoïde. The mixture of experts structure is quite similar to the MLP's. It can appear a bit strange that the mixture of experts has a so simple structure whereas it has a multiple model structure; but this model is based on a combination of a small number of linear models, and thus, the visual complexity of the final prediction stays quite low.

The range of variation of the data is also worth to be noticed. The global SVR is unable to generate extreme values for its prediction while the other methods are. The local SVR is even able to reach very high values on specific hot spots, while the MLP and the mixture of experts are able to predict those high and low values over large areas.

5.4.2 Omni-Directional Variograms of Dense Grid Estimations

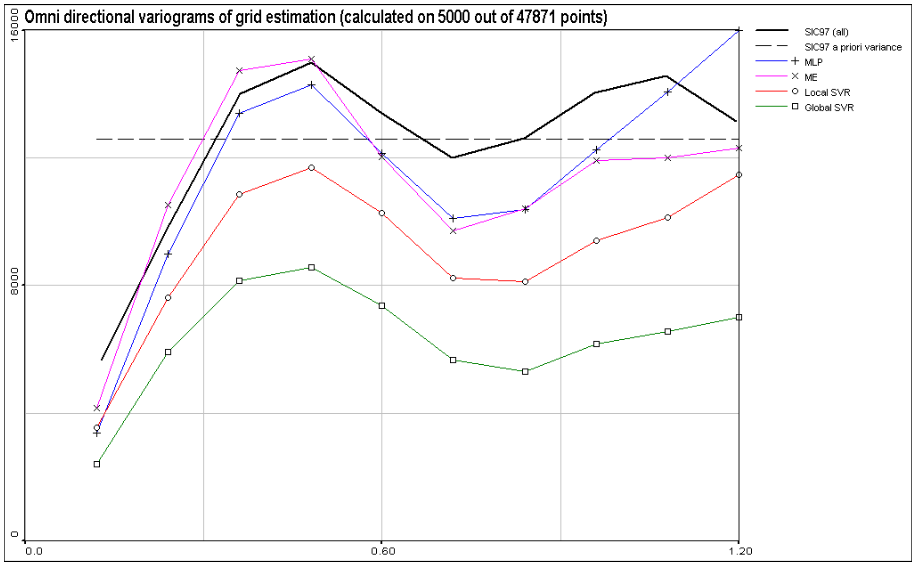


Figure 10: Omni-directional semi-variogram of large grid prediction. The variograms of the four models used to predict the 47871 grid points are represented with the SIC97 data variogram for comparison.

The direct consequence of this variability is represented in the omni-directional variograms shown on Figure 10. The general behavior is very similar to the one of Figure 8. The only difference is that the overall variability of the data has increased. The most surprising with these curves is that one could expect that, given the very sharp and complex picture generated by the local SVR model, its variogram would have been "higher" (i.e. more variable) than the ones from the other models generating smooth and regular pictures. And interestingly, this is not the case. The reason is that the local SVR is generating fewer extreme values than the mixture of experts or the MLP and thus, the "long" range variability is smaller. The sharpness of the local SVR picture, opposed to the smoothness of the other methods, is visible on the nugget effect: the local SVR's one is higher than for all the other methods, sign of a higher local variability.

The conclusion one can extract from this qualitative comparison is that none of the studied regression models is able to give a realistic behavior of the studied phenomenon. The mixture of experts, the MLP and the global SVR are too smooth, while the local SVR produces discontinuous and highly anisotropic features. Thus, it is necessary to remember that predictions done using machine learning methods, like with any other method, are strongly correlated to the method used. And usually, learning algorithms are focusing more on minimizing general statistics (like the expected mean squared error) than local variances, except when trained to do so.

6 Conclusion

As it has already been experimentally shown in the Machine Learning and Geostatistical fields (among others), local models perform usually better than global ones on non-stationary datasets. The experiments conducted on SIC97 data not only reflect the sensitivity of machine learning methods to small and non representative datasets, but also proves that these methods can be efficiently adapted to deal with such problems, and then give better results.

Further researches are now necessary to build some new machine learning methods, specifically adapted to solve Geostatistical problems when classical methods are unable to do so. Mixture models seems to be an interesting direction to follow in order to complete this task.

For what concern Support Vector Machines, it seems that this algorithm is more efficient to solve classification tasks than regression one, although kernel methods appear to be more interpretable than multilayer perceptron.

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Post plot and variogram pictures were generated with Geostat Office software from Russian Nuclear Safety Institute (IBRAE). SVR calculation was done using Alex Smola's quadratic optimizer `pr_loqo`.

SIC97 data were made available by ai-geostats web site (`http://www.ai-geostats.org`) and Journal of Geographic Information and Decision Analysis (GIDA: `http://publish.uwo.ca/~jmalczew/gida.htm`).

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