A comparison of three learning methods to predict N_2O fluxes and N leaching

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Outline

1. Data and problem
2. Presentation of three learning methods
3. Methodology and results

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Measure of agricultural impact

- **Agriculture** back on the top of agenda of policy makers to fight against the food crisis and to alleviate poverty **but** Intensive farming practices cause a **degradation of the other ecosystem services** essential for human survival;

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- To that aim, a platform has been developed in the EC-project CCAT (Cross-Compliance Assessment Tool) that **calculated the impact of cross-compliance legislations on various indicators (GHG, soil pollution, economic indicators, ...)**;
- **But** platform needs **simplified models which make fast simulations** because, in this case, the biogeochemical model DNDC could not be used directly.

Framework of this study

Selection of HSMU related to **corn culture** (about 20 000 spatial units).
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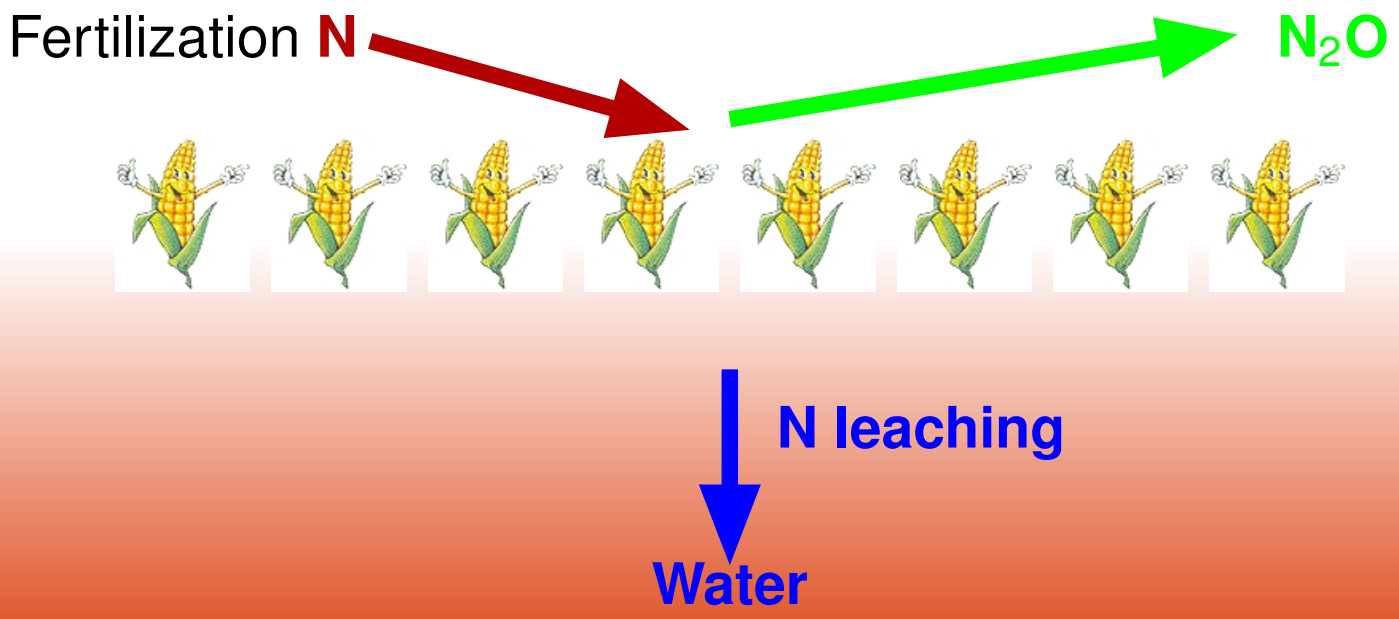

Purpose: Estimation of N_20 and N leaching.

Data

5 data sets corresponding to different scenarios coming from the biogeochemical simulator DNDC-EUROPE.

- S1: Baseline scenario (conventional corn cropping system): 18 794 HSMU
- S2: like S1 without tillage: 18 830 HSMU
- S3: like S1 with a limit in N input through manure spreading at 170 kg/ha y: 18 800 HSMU
- S4: rotation between corn (2y) and catch crop (3y): 40 536 HSMU
- S5: like S1 with an additional application of fertilizer in winter: 18 658 HSMU

Data

11 input variables

- N FR (N input through fertilization; kg/ha y);
- N MR (N input through manure spreading; kg/ha y);
- Nfix (N input from biological fixation; kg/ha y);
- Nres (N input from root residue; kg/ha y);
- BD (Bulk Density; g/cm^3);
- SOC (Soil organic carbon in topsoil; mass fraction);
- PH (Soil PH);
- Clay (Ratio of soil clay content);
- Rain (Annual precipitation; mm/y);
- Tmean (Annual mean temperature; C);
- Nr (Concentration of N in rain; ppm).

Data

2 outputs to estimate from the inputs:

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Comparison of 3 methods:

1. **multi-layer perceptrons** (neural networks): [Bishop, 1995]
2. **Support Vector Machines** (SVM): [Boser et al., 1992]
3. **random forests**: [Breiman, 2001]

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Multilayer perceptrons (MLP)

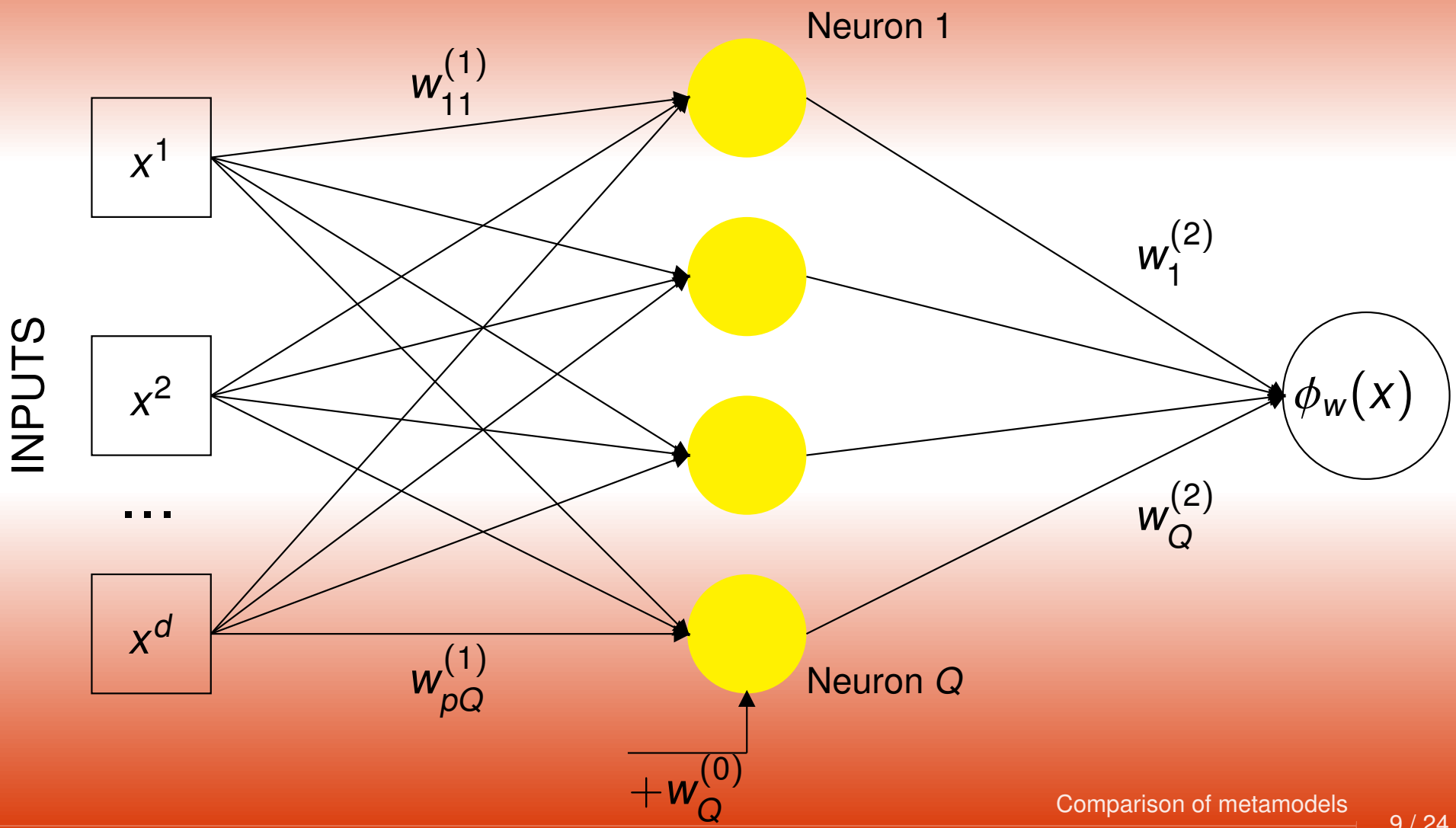
A "one-hidden-layer perceptron" is a function of the form:

$$\Phi_w : x \in \mathbb{R}^d \to \sum_{i=1}^{Q} w_i^{(2)} G\left(x^T w_i^{(1)} + w_i^{(0)}\right) + w_0^{(2)}$$

where:

- the w are the **weights** of the MLP that have to be learned from the learning set;
- G is a given **activation function**: typically, $G(z) = \frac{1-e^{-z}}{1+e^{-z}}$;
- Q is the number of neurons on the hidden layer. It controls the flexibility of the machine. Q is a **hyper-parameter** that is usually tuned during the learning process.

Symbolic representation of MLP



Learning MLP

- **Learning the weights**: w are learned by a **mean squared error minimization** scheme :

$$w^* = \arg\min_w \sum_{i=1}^{N} L(y_i, \Phi_w(x_i)).$$

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- **Tuning of the hyper-parameters, C and Q**: **simple validation** has been used to tune first C and Q.

SVM

SVM is also a error loss with penalization minimization:

1. **Basic linear SVM for regression**: $\Phi_{(w,b)}$ is of the form $x \to w^T x + b$ with (w, b) solution of

$$\arg\min \sum_{i=1}^{N} L_\epsilon(y_i, \Phi_{(w,b)}(x_i)) + \lambda \|w\|^2$$

where

- λ is a regularization (hyper) parameter (to be tuned during the learning process);
- $L_\epsilon(y, \hat{y}) = \max\{|y - \hat{y}| - \epsilon, 0\}$ is an **ϵ-insensitive loss function**

▸ See ϵ-insensitive loss function

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Common kernel: Gaussian kernel

$$K_\gamma(u, v) = e^{-\gamma \|u-v\|^2}$$

is known to have good theoretical properties both for accuracy and generalization.

Learning SVM

- **Learning** (w, b): $w = \sum_{i=1}^{N} \alpha_i K(x_i, .)$ and b are calculated by an exact optimization scheme (quadratic programming). The only step that can be time consumming is the calculation of the kernel matrix:

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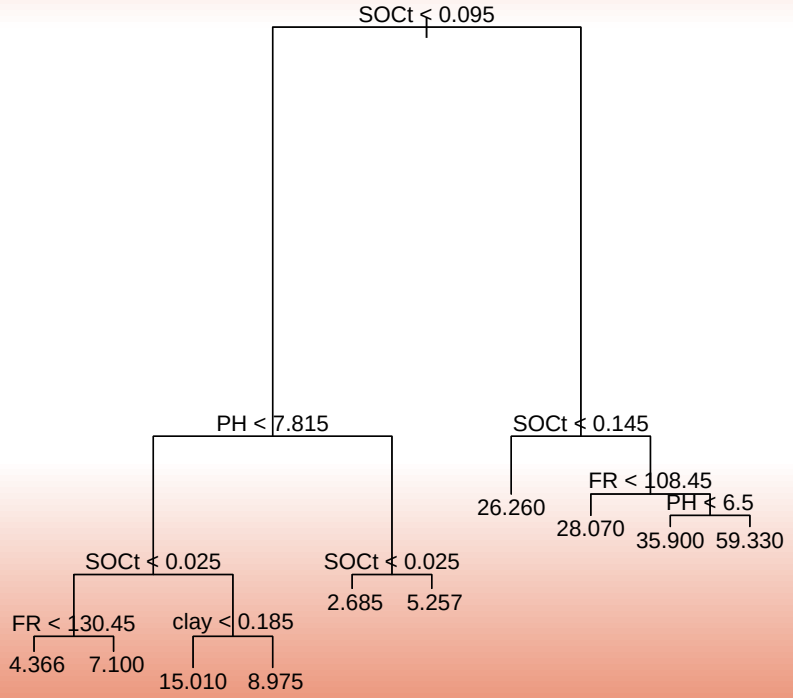
- **Tuning of the hyper-parameters,** $C = 1/\lambda$**,** ϵ **and** γ**: simple validation** has been used. To limit waste of time, ϵ has not been tuned in our experiments but set to the default value (1) which ensured $0.5N$ support vectors at most.

From regression tree to random forest

Example of a regression tree



Each **split** is made such that the two induced subsets have the greatest homogeneity possible.

The **prediction of a final node** is the mean of the Y value of the observations belonging to this node.

Random forest

Basic principle: combination of a large number of under-efficient regression trees (the prediction is the mean prediction of all trees).

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Basic principle: combination of a large number of under-efficient regression trees (the prediction is the mean prediction of all trees). For each tree, **two simplifications** of the original method are performed:

1. A given number of **observations are randomly chosen** among the training set: this subset of the training data set is called in-bag sample whereas the other observations are called out-of-bag and are used to control the error of the tree;
2. For each node of the tree, a given number of **variables are randomly chosen** among all possible explanatory variables.

The best split is then calculated on the basis of these variables and of the chosen observations. The chosen observations are the same for a given tree whereas the variables taken into account change for each split.

Learning a random forest

Random forest are **not very sensitive to hyper-parameters** (number of observations for each tree, number of variables for each split): the default values have been used.

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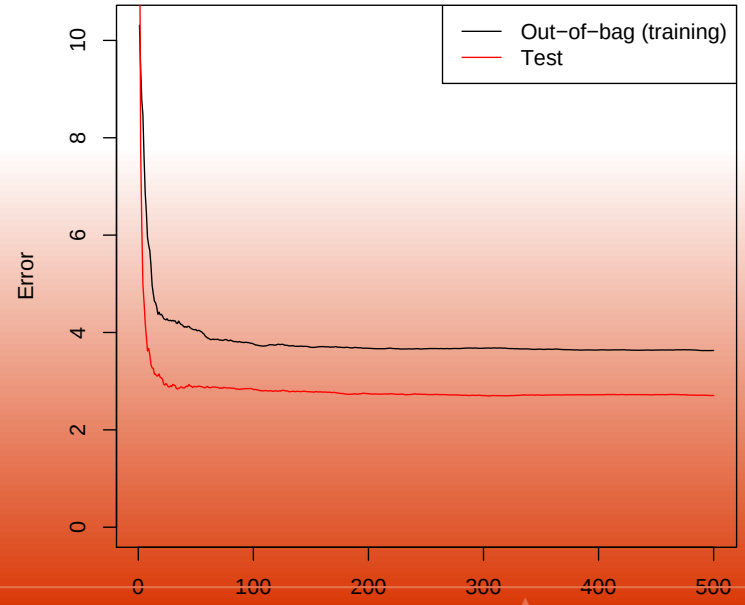
Random forest are **not very sensitive to hyper-parameters** (number of observations for each tree, number of variables for each split): the default values have been used.
The number of trees should be large enough for the mean squared error based on out-of-sample observations to stabilize:



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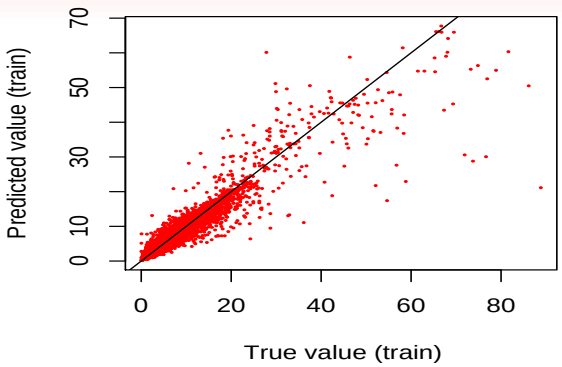
3. The **performances have been calculated** on the basis of the test set: for the test set, predictions have been made from the inputs and compared to the true outputs.

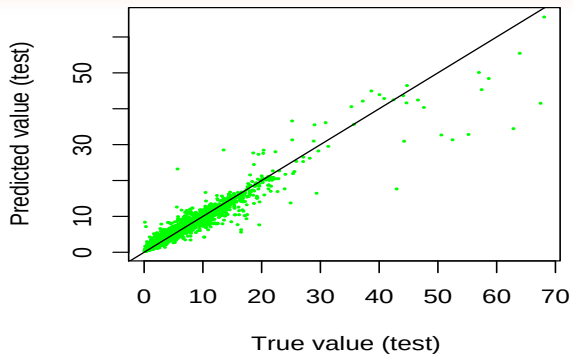
Numerical results

		MLP	RF	SVM	LM
N_2O	Scenario 1	90.7%	**92.3%**	91.0%	77.1%
	Scenario 2	80.3%	**85.0%**	82.3%	62.2%
	Scenario 3	85.1%	**88.0%**	86.7%	74.6%
	Scenario 4	88.6%	**90.5%**	86.3%	78.3%
	Scenario 5	80.6%	**84.9%**	82.7%	42.5%
N leaching	Scenario 1	89.7%	93.5%	**96.6%**	70.3%
	Scenario 2	91.4%	93.1%	**97.0%**	67.7%
	Scenario 3	90.6%	90.4%	**96.0%**	68.6%
	Scenario 4	80.5%	86.9%	**90.6%**	42.5%
	Scenario 5	86.5%	92.9%	**94.5%**	71.1%

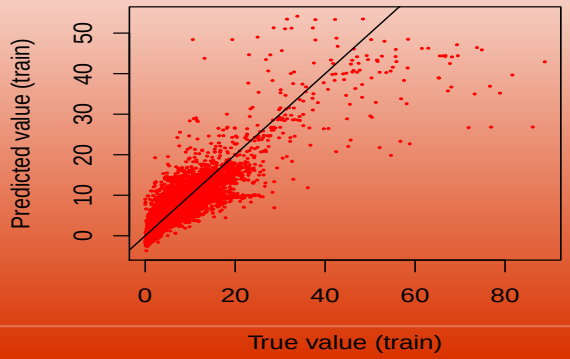
Graphical results

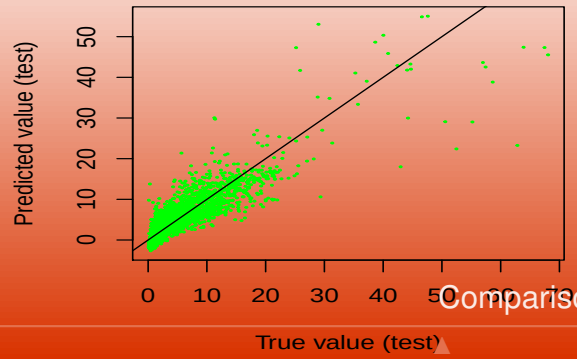
Random forest (S1, N_2O)





Linear model (S1, N_2O)





Further comparisons

	Time for training	Time for using once the model is trained
RF	+ (~ 15 minutes)	= (~ 5 seconds)
SVM	=	- (~ 20 seconds) sensitive to N
MLP	-	+ (~ 1 second) sensitive to d

Times correspond to the prediction for about 20 000 HSMU on a Dell Latitude D830, Intel Core 2DUO 2.2GHz, 2GO RAM, OS Ubuntu Linux 9.10 (and, for RF, to the training of about 15 000 HSMU) with R.

Time for DNDC: around 200 hours by using a desktop computer and around 2 days by using a cluster of computers.

Understanding which inputs are important

Importance: A measure to estimate the importance of the input variables can be defined by:

- for a given input variable randomly permute the input values and calculate the prediction from this new randomly permutated inputs;
- compare the accuracy of these predictions to accuracy of the predictions obtained with the true inputs: the increase of mean squared error is called the importance.

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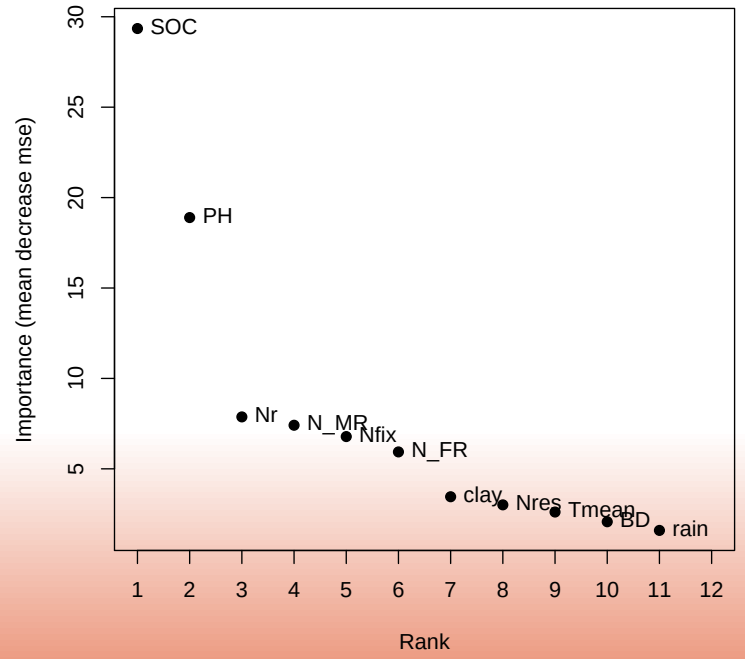
This comparison is made on the basis of data that are not used to define the machine, either the validation set or the out-of-bag observations.

Understanding which inputs are important

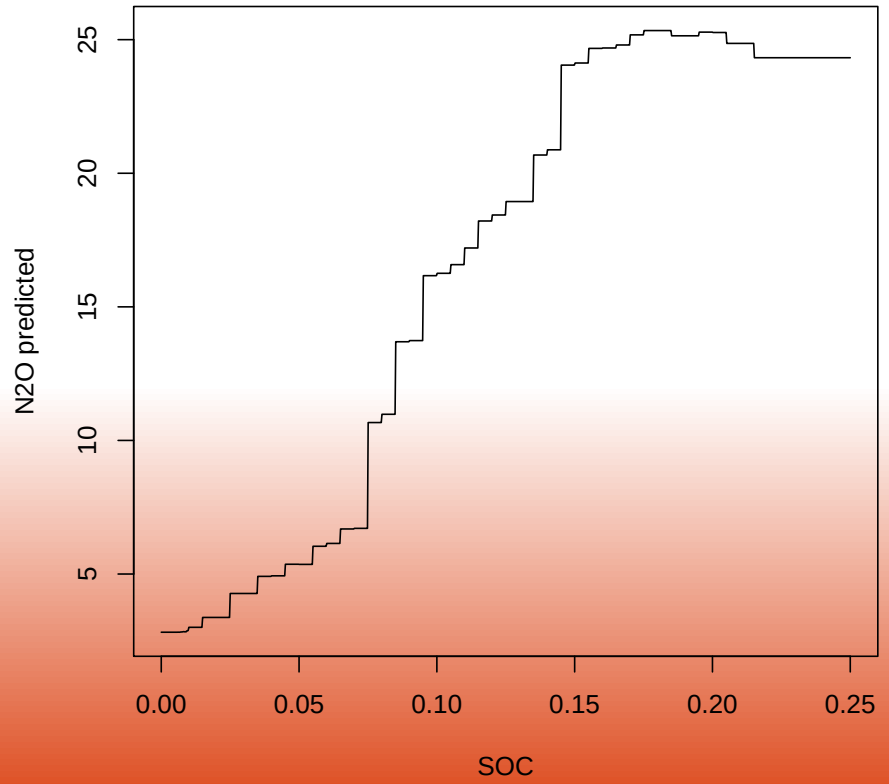
Example (S1, N_2O, RF):



The variables **SOC** and **PH** are the most important for accurate predictions.

Understanding the relation between a given input and the output

Evolution of N_2O in function of the value of SOC



Conclusion and further work

- Learning approaches can provide accurate estimations of the variable of interest much faster than the biogeochemical simulator;
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- Other statistical nonparametric approaches (based on splines) are currently under test.

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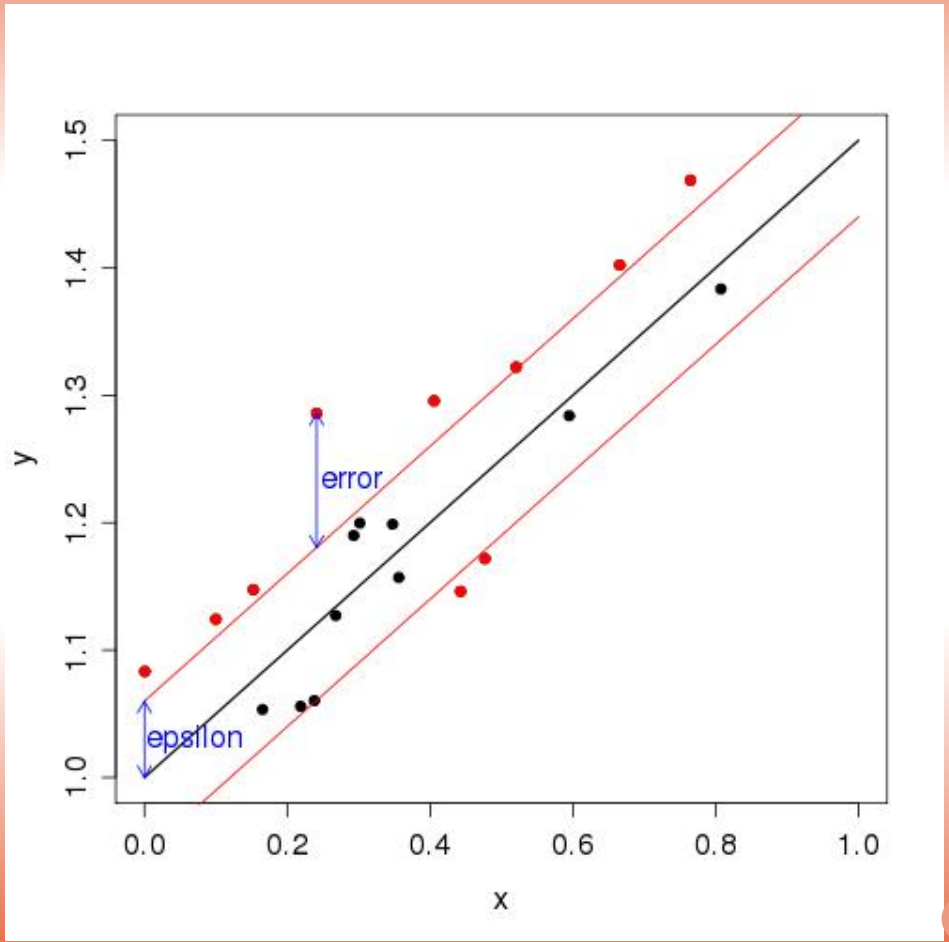
Thank you for your attention.
Questions? Comments?

ϵ-insensitive loss function



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