# FSMLR

**Fast Stepwise Stagewise Multivariateple Linear Regression (FSMLR)** (previous name *Fast Stepwise Multiple Linear Regression*) is a procedure for stepwise stagewise building of linear regression models by means of greedy descriptor selection.

It can be viewed as a special case of the additive regression procedure (regression boosting) specially designed to be compatible with the three-set approach based on the use of three different sets for learning: training set, internal tuning validation set and external test set.

The main configurable parameters are:

- shrinkage – its decrease leads to the decrease of generalization error and increase of the number of required iterations, and
- the relative size of the internal tuning validation set used for stopping descriptor selection procedure.

## Reference

- Zhokhova N, Baskin I, Palyulin V, Zefirov A, Zefirov N. Fragmental descriptors with labeled atoms and their application in QSAR/QSPR studies. Doklady Chemistry. 2007 Dec 1;417(2):282-284.