

The usage of LIBSVM for building SVM-PaDEL model

1. Transport the sdf file to libsvm in the weka.
2. `svm-scale.exe -l 0 -u 1 -s lxr.scale trainset.libsvm>train.scale`
3. `svm-scale.exe -l 0 -u 1 -r lxr.scale testset.libsvm>test.scale`
4. `grid.py train.scale` get the optimum parameters c (32.0) and g (2.0).
5. `svm-train.exe -s 0 -t 2 -c 32.0 -g 2.0 train.scale` get the model
file :train.scale.model
6. `svm-predict.exe test.scale train.scale.model test.predict`