liquidSVM: A Fast and Versatile SVM package

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Abstract

liquidSVM is a package written in C++ that provides SVM-type solvers for various classification and regression tasks. Because of a fully integrated hyper-parameter selection, very carefully implemented solvers, multi-threading and GPU support, and several built-in data decomposition strategies it provides unprecedented speed for small training sizes as well as for data sets of tens of millions of samples. Besides the C++ API and a command line interface, bindings to R, MATLAB, Java, Python, and Spark are available. We present a brief description of the package and report experimental comparisons to other SVM packages.

Keywords: C++, Support Vector Machine, non-parametric classification, non-parametric regression, CUDA, open source, R, Java, MATLAB, Python, Spark

1. Introduction

Support vector machines (SVMs) and related kernel-based learning algorithms are a well-known class of machine learning algorithms, for which a couple of very popular implementations such as SVMlight [Joachims (1999)] and libsvm [Chang and Lin (2011)] as well as some recent packages for large-scale data sets [Tachetti et al. (2013); Djuric et al. (2013); Claesen et al. (2014)] already exist. Despite this, training SVMs is still relatively costly, in particular if it comes to very large data sets and/or hyper-parameter selection. In addition, most packages do not include solvers for more involved estimation problems such as quantile/expectile regression or classification with a constraint on the false alarm rate. The goal of liquidSVM, which is licensed under AGPL 3.0, is to address these issues. In a nutshell, the key features of liquidSVM are:

- Fully integrated hyper-parameter selection based on cross validation
- Extreme speed on both small and large data sets
- Inclusion of a variety of different classification and regression scenarios
- Good default values and high flexibility for experts
- Flexible user interface ranging from a C++ API and a command line version to bindings for R, MATLAB, Java, Python, and Spark

The main software package can be obtained from http://www.isa.uni-stuttgart.de/software and the bindings are packaged under the respective directories /R/matlab/java/python and /spark, resp. liquidSVM has been tested on several versions of Linux and MacOS X, as well as on Windows 8. For the latter two systems pre-compiled binaries are provided, too.
2. Software Description

In liquidSVM an application cycle is divided into a training phase, in which various SVM models are created and validated, a selection phase, in which the SVM models that best satisfy a certain criterion are selected, and a test phase, in which the selected models are applied to test data. These three phases are based upon several components, which can be freely combined. In the following, we briefly describe the four most important components:

**Solvers.** The solvers create SVM models \( f_{D,\lambda,\gamma} \) by solving

\[
 f_{D,\lambda,\gamma} = \arg\min_{f \in H_\gamma} \lambda \|f\|_H^2 + \frac{1}{n} \sum_{i=1}^{n} L_w(y_i, f(x_i)).
\]  

(1)

Here \( \lambda > 0 \) is a regularization parameter, \( H_\gamma \) is a reproducing kernel Hilbert space with kernel \( k_\gamma \) and kernel parameter \( \gamma > 0 \), \( D = ((x_1, y_1), \ldots, (x_n, y_n)) \) is a labeled data set, and \( L_w \) is a loss function with weight parameter \( w > 0 \). Currently, liquidSVM include solvers for the (weighted) hinge loss used for classification, the least squares loss used for mean regression, the pinball loss used for quantile regression, and the asymmetric least squares loss used for expectile regression. Moreover, the standard Gaussian RBF kernel and the Laplacian kernel are implemented and it is possible to add own normalized kernels.

**Hyper-Parameter Selection.** The problem \( (1) \) has the free parameters \( \lambda \) and \( \gamma \), and in some situations, also \( w \). liquidSVM automatically determines good values for these parameters by performing \( k \)-fold cross validation (CV) over an (adaptive) grid of candidate values. The user can choose between different fold generation methods and can also determine the candidate grid and the loss function used on the validation fold. In addition, the user can decide, whether one SVM model or \( k \) SVM models are created during the selection phase and, if applicable, how these \( k \) models are combined during the test phase. To speed up the CV, the required kernel matrices may be re-used and all solvers contain advanced warm start options. By default, the most time efficient combinations are picked.

**Managing Working Sets.** Some learning scenarios such as one-versus-all (OvA) multiclass classification require to solve \( (1) \) for a couple of different subsets \( D \) of the full data set. In liquidSVM each such data set is associated to a task. Moreover, a well-known strategy to speed up training is to split the data into smaller parts or cells, see e.g. Bottou and Vapnik (1992), Vapnik and Bottou (1993). Currently, liquidSVM offers to create tasks according to OvA, AvA, as well as to weighted classification and quantile/expectile regression. In addition, several methods to create random or spatially defined cells are implemented. Different task and cell creation methods can be freely combined and at the end, hyper-parameter selection as described above is performed on each resulting cell.

**User Interfaces and Pre-defined Learning Scenarios.** Besides the C++ class API for experienced users, liquidSVM also has a command line interface (CLI) as well as bindings to R, MATLAB, Python, and Java. Both the CLI and the bindings contain routines for various standard learning scenarios such as: (weighted) binary classification, multiclass classification (both AvA and OvA), Neyman-Pearson-type classification, least squares regression, quantile regression, and expectile regression. These routines also have a simplified interface to facilitate a fast and easy access to the functionality of liquidSVM.
3. Implementation Details

liquidSVM is written in C++ and its main functionality is accessible through a small number of high-level C++ classes. The code is divided into four parts: a) SVM independent code for I/O-operations, data set manipulations, and generic k-fold CV, b) SVM related code such as the core solvers, c) code for some extra CLI tools, and d) code related to the bindings.

The routines for computing the kernel matrices and for evaluating the SVM models on the test data are parallelized to run on multiple cores and for Linux, Cuda implementations of these routines do also exist. Time critical inner loops may be vectorized with the following instruction sets: SSE2, AVX, and AVX2. When compiling liquidSVM under Linux or MacOS X the best instruction set for the current machine is chosen, while in the bindings we additionally offer an explicit compilation with SSE2.

All currently available solvers are based on the design principles for the hinge loss solver described by Steinwart et al. (2011). For the least squares and quantile solver, the corresponding modifications were straightforward, while for the expectile solver more care was necessary, see Farooq and Steinwart (2017).

All bindings share a common C-interface to liquidSVM’s C++ code. They perform all operations in-memory and in a single process, which may control several threads.

4. Benchmarks

To illustrate the speed of liquidSVM we report some comparisons to other available implementations. Here, we only give a brief summary of our results, more extensive experiments as well as further details can be found in the appendix in Section B. Except in the comparison to GURLS, we only considered binary classification since this is the common denominator of the considered implementations. In our experiments we performed 5-fold CV to select the hyper-parameters from a $10 \times 11$-grid suggested by libsvm, and for liquidSVM we additionally considered its default $10 \times 10$-grid. For packages not containing a CV routine, we manually implemented it by wrapping loops.

For small data sets of size $n = 4000$ we considered three implementations that have an R-interface, namely: package e1071, which binds to libsvm, package klaR (Weihs et al. 2005), which wraps SVMlight, and package kernlab (Karatzoglou et al. 2004), which is implemented entirely in R. The corresponding results, which are summarized in Table 1, show that even with a single thread liquidSVM is more than an order of magnitude faster. Similarly, Table 2 shows that liquidSVM is between 7 and 35 times faster than GURLS (Tacchetti et al. 2013) on four multiclass data sets of size $n \leq 10000$.

For medium-sized data sets with $n \leq 280000$ we considered the following two implementations that allow a partition of the training set into cells: BudgetedSVM (Djuric et al. 2013) and EnsembleSVM (Claesen et al. 2014). Both have a parameter $k$, which can be compared to our cell size. In Table 3 we report the results for $k = 1000$ (results for $k = 500, 3000$ can be found in the appendix). It turns out that liquidSVM is in many cases two orders of magnitude faster, and in most cases it also achieves a significant reduction of the test error.

Finally, for large training sets up to around 30 million samples we performed experiments on a Spark cluster, see Table 4. Here, we actually achieved in most cases a slightly super-linear speed-up compared to the single-node run, since less overhead was created.
Table 1: Cross validation time for small (n=4000) data sets. The times are given relative to our fully optimized implementation on the hyper-parameter grid of libsvm, for which we also present the absolute time in seconds. Times are averaged over 10 independent repetitions. liquidSVM (outer cv) uses e1071::tune and solves in every grid-point a single SVM. SVMlight is quite slow here due to disk accesses in the wrapper. In these experiments liquidSVM is single-threaded, the other implementations do not support multi-threading. The test errors are comparable (see Table 7 in the Appendix).

Table 2: Comparison to GURLS for multi-class classification. For our implementations we used OvA with the least-squares solver and no cell splitting. GURLS has an internal parameter selection for the cost parameter while the kernel parameter was set by their heuristic involving the lower quartile of the distance matrix values. Both implementations used full multi-threading (6 physical for GURLS, 12 logical for GURLS).

Table 3: Benchmarks for splitting mid-sized data sets with cell size 1000. The left side presents single-threaded training times (relative to liquidSVM) including 5-fold CV, and on the right-hand side the corresponding classification errors (in %) can be found. Overlap uses our solver but with overlapping instead of mutually disjoint cells. Our errors are almost always significantly better, while in many cases the speed-up is two orders of magnitudes.

Table 4: Benchmarks on a Spark cluster with 14 workers, each using 6 threads. The data was first split into coarse cells of size approximately 20000 and every cell was collected on a single worker. Then each such coarse cell was solved locally using fine cells of size at most 2000. The single node experiments are taken from [Thomann et al. 2016] using the command line version on the same machines using 6 threads. The speedup is in most cases super-linear since less overhead is created. All times include 5-fold CV on our 10×10-grid.
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Appendix A. Usage

A.1 Command Line Interface

For Linux download [liquidSVM.tar.gz](http://www.isa.uni-stuttgart.de/R) and use the following commands to compile and train and test a multi-class SVM on our banana data set with display verbosity 1 and using 2 threads:

```bash
tar xzf liquidSVM.tar.gz
cd liquidSVM
make all
cd scripts
./mc-svm.sh banana-mc 1 2
```

A.2 R

You can use the following example:

```r
install.packages("liquidSVM", repos="http://www.isa.uni-stuttgart.de/R")
library(liquidSVM)
d <- liquidData('banana-mc')  # load the multi-class banana data set
model <- mcSVM(Y ~ ., d$train, display=1, threads=2)
result <- test(model, d$test)
```

More information can be found in the [demo](http://www.isa.uni-stuttgart.de/R) and [documentation](http://www.isa.uni-stuttgart.de/R) vignettes online. Also consider the manuals for the package ?liquidSVM or for the commands ?lsSVM, ?mcSVM, etc.

A.3 Java

For installation download [liquidSVM-java.zip](http://www.isa.uni-stuttgart.de/R) and unzip it. The classes are all in package de.uni_stuttgart.isa.liquidsvm and an easy example is:

```java
SVM s = new LS(trainX, trainY, new Config().display(1).threads(2));
ResultAndErrors result = s.test(testX, testY);
```

If this is implemented in file Example.java this can be compiled and run using

```bash
javac -classpath liquidSVM.jar Example.java
java -Djava.library.path=. -cp .:liquidSVM.jar Example
```

A.4 MATLAB/Octave

For installation download the Toolbox [liquidSVM.mltbx](http://www.isa.uni-stuttgart.de/R) and install it in MATLAB by double clicking it. Then you can use it like:

```matlab
makeliquidSVM native
load data
model = mcSVM(banana_mc_train_x, banana_mc_train_y, 'DISPLAY','1','THREADS','2');
model.test(banana_mc_test_x, banana_mc_test_y);
```

If the training labels are categorical they are transparently converted to integer labels and in this case, if no learning scenario is specified, binary or multi-class classification is performed by default. The code also works in Octave if you use [liquidSVM-octave.zip](http://www.isa.uni-stuttgart.de/R).
A.5 Python

Install using

```
pip install --user \\n   http://www.isa.uni-stuttgart.de/software/python/liquidSVM-python.tar.gz
```

this also will install numpy if it is not available yet. Then in Python the package is used as:

```python
from liquidSVM import *
model = mcSVM(iris, iris_labs, display=1, threads=2)
result, err = model.test(iris, iris_labs)
```

A.6 Spark

Download [liquidSVM-spark.zip](http://www.isa.uni-stuttgart.de/software/python/liquidSVM-spark.zip) and unzip it and issue:

```
make lib
export LD_LIBRARY_PATH=.:$LD_LIBRARY_PATH
$SPARK_HOME/bin/spark-submit --master local[*] \
   --class de.uni_stuttgart.isa.liquidsvm.spark.liquidSVMsparkApp \
   liquidSVM-spark.jar covtype.full.10000
```

If you have configured Spark to be used on a cluster with Hadoop use:

```
hdfs dfs -put data/covtype-full.train.csv data/covtype-full.test.csv .
make lib
$SPARK_HOME/spark-submit --files ../libliquidsvm.so \
   --conf spark.executor.extraLibraryPath= . \
   --conf spark.driver.extraLibraryPath= . \
   --class de.uni_stuttgart.isa.liquidsvm.spark.liquidSVMsparkApp \
   --num-executors 14 liquidSVM-spark.jar covtype-full
```

Appendix B. Details and further benchmarks

In this section we present more extensive benchmarks and give some technical details. First consider Table 5 for an overview of all considered implementations.

Let us first give some general details on the hyper-parameter grids we used for cross-validation. By `libsvm` grid we mean here the $10 \times 11$ grid given by

$$
\gamma \in \{2^3, 2, 2^{-1}, 2^{-3}, 2^{-5}, 2^{-7}, 2^{-9}, 2^{-11}, 2^{-13}, 2^{-15}\},
$$

$$
cost \in \{2^{-5}, 2^{-3}, 2^{-1}, 2, 2^3, 2^5, 2^7, 2^9, 2^{11}, 2^{13}, 2^{15}\},
$$

which is suggested by the default values in the file `tools/grid.py` of `libsvm`. For `liquidSVM` we performed experiments both on this grid and on our default $10 \times 10$ geometrically spaced hyper-parameter grid where the endpoints are scaled to accommodate the number of samples in every fold, the cell size, and the dimension.

B.1 Small-sized data sets

Every data set was split into 10 training sets of size $n \in \{1000, 2000, 4000\}$ and 10 test sets. Based on the training a scaling was determined and both training and test set were normalized by that. We did all the computation in R and used package `e1071` which binds
Table 5: Features of the different implementations we consider here. In the top are the implementations we used for small-sized data sets, in the middle those for medium-sized, and in the bottom our.

Table 6: Cross validation time for different implementations on small-sized data sets. Times are means of 10 independent repetitions and all involve 5-fold cross-validation on a 10x11 grid – only our optimized version uses its usual 10x10 grid. liquidSVM (outer cv) uses e1071::tune and solves in every grid-point a single SVM. SVMlight is quite slow here due to need of disk access in the wrapper. liquidSVM here is single-threaded, the others do not support multi-threading.

We also reproduced some of the results of GURLS (Tacchetti et al., 2013). As they do not provide a command line interfaces, we had to adapt their example C++ program to use their library in Version 2.0. After communication with the authors we used their internal parameter selection for the cost parameters and their heuristic for the kernel parameter...
(lower quartile of distances). Our reproduced runtimes using their software are about factor 40 faster than their reported ones and we attribute this to the following factors: it seems their written times are reported for MATLAB where we used their C++ version, we used 6 threads, and our cpu was clocked 37% higher.

### B.2 Medium-sized data sets

We considered several implementations that use a random chunk approach to scale SVMs. Based on the training data a scaling was determined and both training and test set were normalized by that. Then we used Bash scripts to perform cross validation. We used an Intel\textsuperscript{®} Core\textsuperscript{TM} i7-3930K cpu at 3.20GHz with 64GB memory and AVX running Debian Linux. The results for cell sizes $k = 500, 3000$ are in Tables 8 and 9 (and we also repeat here those for $k = 1000$).

It is commendable, that BudgetedSVM publish on their web page\footnote{http://www.dabi.temple.edu/budgetedsvm/docs/run_budgetedsvm_algs.m} the concrete hyperparameters they were using for experiments (at least for $k = 500$). However they not describe, how they found them. Our CV found for WEbspAM the same cost 0.125, however we found $\gamma = 8$ to have better validation error than their $\gamma = 16$ (which is in their definition of the kernel function actually $\tilde{\gamma} = 32$). We also tried out their BSGD-variant, however (at least for $k = 500$) this was always 10 times slower than their LLSVM-variant and hence would need much more time to finish. We used Version 1.1.

EnsembleSVM (version 2.0) has a nice interface to mask sets for training and validation splits. Sadly, there is no out of the box script to perform cross-validation only an example on their homepage.

A bit annoyingly, on the $10 \times 11 \times 5$ grid training was hanging some times, and one had to kill the process (after holidays we found out that on solver had run without convergence for several days). To remain comparable, we subtracted the whole excess time!

|       | liquidSVM | (libsvm grid) | libsvm | kernlab | SVMlight |
|-------|-----------|---------------|--------|---------|----------|
| BANK-MARKETING | 0.1115 | 0.1111 | 0.1110 | 0.1113 | 0.1153 |
| COD-RNA | 0.0446 | 0.0454 | 0.0434 | 0.0452 | 0.0497 |
| COVTYPE | 0.2526 | 0.2474 | 0.2580 | 0.2540 | 0.2506 |
| THYROID-ANN | 0.0534 | 0.0511 | 0.0488 | 0.0477 | 0.0460 |
|       | liquidSVM | (libsvm grid) | libsvm | kernlab | SVMlight |
| BANK-MARKETING | 0.1090 | 0.1085 | 0.1086 | 0.1087 | 0.1160 |
| COD-RNA | 0.0416 | 0.0431 | 0.0414 | 0.0416 | 0.0485 |
| COVTYPE | 0.2284 | 0.2263 | 0.2315 | 0.2324 | 0.2440 |
| THYROID-ANN | 0.0512 | 0.0484 | 0.0457 | 0.0464 | 0.0464 |
|       | liquidSVM | (libsvm grid) | libsvm | kernlab | SVMlight |
| BANK-MARKETING | 0.1070 | 0.1066 | 0.1065 | 0.1065 | 0.1165 |
| COD-RNA | 0.0401 | 0.0413 | 0.0391 | 0.0393 | 0.0482 |
| COVTYPE | 0.2038 | 0.2055 | 0.2074 | 0.2067 | 0.2411 |
| THYROID-ANN | 0.0457 | 0.0458 | 0.0429 | 0.0433 | 0.0803 |

Table 7: Mean classification errors for different implementations on small-sized data sets.
Table 8: Cross validation time (in min.) for medium-sized data sets. In the left part the times are single-threaded, in the right part, they are with 6 threads. For $k = 3000$ the others only use a $9 \times 10$-grid.

| $k = 500$ | liquidSVM (libsvm grid) | Overlap | Bsvm | Esvm | liquidSVM (libsvm grid) | Overlap | Esvm |
|-----------|-------------------------|---------|------|------|-------------------------|---------|------|
| covtype.10000 | 0.1 | 0.1 | 0.5 | 33.7 | 17.4 | 0.1 | 0.1 | 0.5 | 9.0 |
| covtype.40000 | 0.6 | 0.4 | 4.1 | 138.4 | 37.8 | 0.5 | 0.4 | 4.3 | 28.9 |
| covtype.100000 | 1.4 | 0.9 | 11.8 | 305.1 | 94.0 | 1.2 | 0.9 | 11.4 | 65.1 |
| ijcnn1 | 0.4 | 0.4 | 9.9 | 140.0 | 27.7 | 0.4 | 0.4 | 11.7 | 24.1 |
| webspam | 4.7 | 4.9 | 293.5 | 997.5 | 775.4 | 4.3 | 4.5 | 275.1 | 754.0 |

| $k = 1000$ | liquidSVM (libsvm grid) | Overlap | Bsvm | Esvm | liquidSVM (libsvm grid) | Overlap | Esvm |
|-----------|-------------------------|---------|------|------|-------------------------|---------|------|
| covtype.10000 | 0.2 | 0.1 | 0.5 | 102.1 | 7.9 | 0.2 | 0.1 | 0.3 | 13.3 |
| covtype.40000 | 0.8 | 0.6 | 4.9 | 372.9 | 41.2 | 0.6 | 0.4 | 3.1 | 26.3 |
| covtype.100000 | 2.0 | 1.4 | 16.5 | 842.8 | 172.1 | 1.4 | 0.9 | 9.9 | 136.6 |
| ijcnn1 | 0.7 | 0.6 | 5.3 | 358.3 | 32.4 | 0.4 | 0.5 | 2.9 | 23.9 |
| webspam | 6.2 | 6.2 | 572.9 | 2545.4 | 2961.5 | 3.9 | 4.0 | 295.0 | 2663.4 |

| $k = 3000$ | liquidSVM (libsvm grid) | Overlap | Bsvm | Esvm | liquidSVM (libsvm grid) | Overlap | Esvm |
|-----------|-------------------------|---------|------|------|-------------------------|---------|------|
| covtype.10000 | 0.4 | 0.3 | 0.8 | 690.4 | 343.4 | 0.2 | 0.1 | 0.3 | 83.6 |
| covtype.40000 | 1.7 | 1.3 | 5.1 | 1711.0 | 388.1 | 0.8 | 0.4 | 2.0 | 122.0 |
| covtype.100000 | 4.2 | 3.5 | 29.7 | 3513.3 | 518.6 | 1.8 | 1.1 | 11.0 | 250.7 |
| ijcnn1 | 1.6 | 1.7 | 2.7 | 1841.2 | 190.1 | 0.5 | 0.6 | 0.8 | 81.5 |
| webspam | 12.6 | 12.4 | 2519.7 | 12993.8 | 3052.7 | 4.4 | 4.3 | 683.7 | 2370.5 |

Table 9: Classification errors (in %) for different implementations on medium-sized data sets. BudgetedSVM (LLSVM) published for WEbspam error rates of 3.46, 2.60, and 1.99, resp. (Djuric et al., 2013). For EnsembleSVM published for COVTYPE and IJCNN1 error rates of 11%, and 9% resp. (Claesen et al., 2014). For $k = 3000$ the others only use a 9 \times 10-grid.
B.3 Large-sized data sets

As architecture, we used Intel® Xeon® CPUs (E5-2640 0 at 2.50GHz, May 2013) with Ubuntu Linux. There were two NUMA-sockets each with a CPU having 6 physical cores with 128GB memory and AVX. We thank the Institute of Mathematics at the University of Zurich for providing us access to those machines.

Let us repeat here our description from Thomann et al. (2016): The data set was saved on a Hadoop distributed file system on one master and 7 worker machines of the above type. In a first step, the data was split into coarse cells of estimated size 20000 by the following procedure. A subset of the training data was sampled and sent to the master machine where 300–8000 centres were found and these centres were sent back to the worker machines. Now each worker machine could assign locally to every of it’s samples the coarse cell in the Voronoi sense. Finally a Spark-shuffle was performed: Every cell was assigned to one of the workers and all its samples were sent to that worker.

In the second step every such coarse cell–now being on one physical machine–was used for training by our C++ implementation discussed above: this in particular means that each coarse cell was again split into fine cells of size 2000. Obviously this now was done in parallel on all worker nodes. The test set was also split into the coarse cells and then by our implementation further into fine cells for prediction.

The single node times and errors (as well as the above two-paragraph description) are from Thomann et al. (2016). For these the command line interface was used on the same machines. Hence they have much more overhead in terms of disk access and retraining. This explains the super-linear speed-up, even though for the Spark-version there has to be done some shuffling over an Ethernet-LAN.

Appendix C. Benchmarks for liquidSVM configurations

liquidSVM can be configured extensively. They are described in the documentation of the software. We selected some of those and performed experiments for the small-sized data sets. The selection is for the following parameters:

- **threads**: Controls the number of threads in the kernel evaluations
- **grid_choice=0**: our standard 10×10 hyper-parameter grid.
- **grid_choice=1**: a 15×15 hyper-parameter grid
- **grid_choice=2**: a 20×20 hyper-parameter grid
- **adaptivity_control**: selects adaptively a subset of the hyper-parameter grid
- **voronoi**: value 5 uses a overlapping decomposition into cells, value 6 specifies our recursive partitioning scheme. The optional second parameter specifies the maximal cell size (default 2000).

The training times and classification errors are given in Tables 10–13. There are more configurations that are useful to control time and memory consumption however we did not benchmark them here.

**Architecture.** Native code can be compiled using several levels of single-instruction-multiple-data (SMD) instruction sets: SSE2, AVX, AVX2. Compiling with native will select the highest available setting. All of the experiments up to here were compiled with native. We invested some effort to also compile the other implementations using native yet they
**Table 10:** On the left: training time for different configurations relative to threads=4. On the right: classification errors in %. They are all averaged over 10 repetitions (n=1000).

| threads=1 | BASE-MARKETING | CORD-INA | COTYPE | THYROID-ANN |
|-----------|----------------|----------|--------|-------------|
|           | 1.18           | 1.23     | 1.19   | 1.20        | 11.06  | 4.32 | 24.51 | 5.17 |
| threads=2 | 1.15           | 1.20     | 1.17   | 1.17        | 11.14  | 4.46 | 24.40 | 5.47 |
| threads=3 | 1.06           | 1.05     | 1.05   | 1.06        | 11.04  | 4.44 | 24.87 | 5.32 |
| threads=4 | 1.00           | 1.00     | 1.00   | 1.00        | 11.19  | 4.44 | 24.42 | 5.45 |
| grid_choice=1 | 2.96   | 2.15     | 2.45   | 2.52        | 11.13  | 4.36 | 24.41 | 4.93 |
| grid_choice=2 | 7.03   | 5.61     | 7.51   | 8.31        | 11.19  | 4.44 | 24.45 | 4.71 |
| adaptivity_control=1 | 0.89 | 0.88     | 0.86   | 0.84        | 11.09  | 4.44 | 24.40 | 5.32 |
| adaptivity_control=2 | 0.79 | 0.77     | 0.80   | 0.74        | 11.16  | 4.34 | 24.75 | 5.26 |
| adaptivity_control=2, grid_choice=2 | 3.55 | 2.66     | 2.96   | 3.62        | 11.13  | 4.40 | 24.67 | 5.13 |
| voronoi=5 | 0.99           | 0.99     | 1.00   | 1.01        | 11.12  | 4.49 | 24.72 | 5.17 |
| voronoi=6 | 0.99           | 0.99     | 0.99   | 1.00        | 11.10  | 4.36 | 24.74 | 5.25 |
| voronoi=c(5,1000) | 0.99 | 0.99 | 0.99 | 1.00 | 11.02  | 4.34 | 24.48 | 5.31 |
| voronoi=c(6,1000) | 1.00 | 1.00 | 1.01 | 1.00 | 11.21  | 4.35 | 25.04 | 5.33 |

**Table 11:** On the left: training time for different configurations relative to threads=4. On the right: classification errors in %. They are all averaged over 10 repetitions (n=2000).

| threads=1 | BASE-MARKETING | CORD-INA | COTYPE | THYROID-ANN |
|-----------|----------------|----------|--------|-------------|
|           | 1.67           | 1.81     | 1.59   | 1.64        | 10.84  | 4.11 | 22.83 | 4.94 |
| threads=2 | 1.25           | 1.29     | 1.21   | 1.25        | 10.81  | 4.23 | 22.80 | 4.78 |
| threads=3 | 1.08           | 1.11     | 1.07   | 1.06        | 10.86  | 4.13 | 22.59 | 4.91 |
| threads=4 | 1.00           | 1.00     | 1.00   | 1.00        | 10.84  | 4.31 | 22.78 | 4.75 |
| grid_choice=1 | 2.66 | 2.16     | 2.81   | 2.71        | 10.83  | 4.16 | 22.61 | 4.62 |
| grid_choice=2 | 9.55 | 6.77     | 10.36  | 11.60       | 10.90  | 4.19 | 22.89 | 4.67 |
| adaptivity_control=1 | 0.90 | 0.86 | 0.90 | 0.76 | 10.86  | 4.16 | 22.82 | 4.94 |
| adaptivity_control=2 | 0.76 | 0.76 | 0.78 | 0.66 | 10.90  | 4.13 | 22.59 | 4.97 |
| adaptivity_control=2, grid_choice=2 | 4.28 | 2.84 | 3.78 | 3.85 | 10.81 | 4.16 | 22.69 | 4.60 |
| voronoi=5 | 1.00           | 1.01     | 0.99   | 0.97        | 10.83  | 4.21 | 22.62 | 4.80 |
| voronoi=6 | 1.02           | 1.01     | 1.01   | 0.95        | 10.83  | 4.24 | 22.70 | 4.81 |
| voronoi=c(5,1000) | 0.89 | 1.20 | 0.85 | 0.93 | 11.06  | 4.25 | 22.98 | 5.23 |
| voronoi=c(6,1000) | 0.70 | 0.75 | 0.67 | 0.65 | 11.11 | 4.36 | 22.87 | 5.41 |
| threads=1 | BANK-MARKETING | COD-RNA | COTYPE | COTHYROID-ANN | 10.71 | 4.04 | 20.31 | 4.57 |
| threads=2 | 1.20 | 1.25 | 1.19 | 1.24 | 10.67 | 4.12 | 20.33 | 4.63 |
| threads=3 | 1.05 | 1.08 | 1.05 | 1.07 | 10.73 | 4.05 | 20.35 | 4.70 |
| threads=4 | 1.00 | 1.00 | 1.00 | 1.00 | 10.75 | 4.04 | 20.22 | 4.68 |
| grid_choice=1 | 2.74 | 2.13 | 3.02 | 3.01 | 10.76 | 4.15 | 20.53 | 4.55 |
| grid_choice=2 | 11.11 | 7.23 | 12.38 | 15.03 | 10.65 | 4.05 | 20.52 | 4.57 |
| adaptivity_control=1 | 0.88 | 0.90 | 0.89 | 0.72 | 10.70 | 4.08 | 20.40 | 4.69 |
| adaptivity_control=2 | 0.73 | 0.75 | 0.79 | 0.60 | 10.73 | 4.01 | 20.27 | 4.57 |
| adaptivity_control=2, grid_choice=2 | 4.08 | 2.67 | 3.45 | 2.92 | 10.66 | 4.16 | 20.61 | 4.52 |
| voronoi=5 | 0.71 | 0.90 | 0.74 | 0.76 | 10.83 | 4.06 | 20.57 | 4.85 |
| voronoi=6 | 0.45 | 0.50 | 0.49 | 0.44 | 10.84 | 4.06 | 20.47 | 4.87 |
| voronoi=c(5,1000) | 0.66 | 0.74 | 0.53 | 0.85 | 10.86 | 4.03 | 20.57 | 4.77 |
| voronoi=c(6,1000) | 0.38 | 0.44 | 0.35 | 0.35 | 10.92 | 4.09 | 20.74 | 5.06 |

Table 12: On the left: training time for different configurations relative to $\text{threads}=4$. On the right: classification errors in %. They are all averaged over 10 repetitions ($n=4000$).

| threads=1 | BANK-MARKETING | COD-RNA | COTYPE | COTHYROID-ANN | 10.55 | 4.00 | 18.86 |
| threads=2 | 1.19 | 1.25 | 1.17 | 1.17 | 10.61 | 3.97 | 18.85 |
| threads=3 | 1.06 | 1.08 | 1.05 | 1.05 | 10.58 | 3.98 | 18.75 |
| threads=4 | 1.00 | 1.00 | 1.00 | 1.00 | 10.54 | 3.98 | 18.57 |
| grid_choice=1 | 2.85 | 2.18 | 3.17 | 3.17 | 10.56 | 4.03 | 18.75 |
| grid_choice=2 | 12.20 | 7.45 | 13.77 | 13.77 | 10.66 | 4.00 | 18.63 |
| adaptivity_control=1 | 0.88 | 0.91 | 0.87 | 0.87 | 10.57 | 4.00 | 18.80 |
| adaptivity_control=2 | 0.75 | 0.78 | 0.79 | 0.79 | 10.55 | 3.99 | 18.77 |
| adaptivity_control=2, grid_choice=2 | 4.25 | 2.58 | 2.80 | 2.80 | 10.59 | 4.01 | 18.73 |
| voronoi=5 | 0.55 | 0.60 | 0.52 | 0.52 | 10.69 | 3.95 | 18.84 |
| voronoi=6 | 0.32 | 0.34 | 0.31 | 0.31 | 10.80 | 3.98 | 18.91 |
| voronoi=c(5,1000) | 0.49 | 0.65 | 0.50 | 0.50 | 10.79 | 3.94 | 18.94 |
| voronoi=c(6,1000) | 0.26 | 0.28 | 0.25 | 0.25 | 10.96 | 4.09 | 19.29 |

Table 13: On the left: training time for different configurations relative to $\text{threads}=4$. On the right: classification errors in %. They are all averaged over 10 repetitions ($n=6000$).
did not benefit. For ours we report results for different compiler settings in Tables 14–17. Obviously native here gives AVX2.

| threads=1   | threads=2   | threads=3   | threads=4   | grid_choice=1 | grid_choice=2 | adaptivity_control=1 | adaptivity_control=2 | adaptivity_control=2, grid_choice=2 | voronoi=5 | voronoi=6 | voronoi=c(5,1000) | voronoi=c(6,1000) |
|-------------|-------------|-------------|-------------|---------------|-----------------|----------------------|----------------------|-------------------------------------|-----------|-----------|-------------------|-------------------|
|             |             |             |             |               |                 |                      |                      |                                     |           |           |                   |                   |
| bank-marketing | bank-marketing | bank-marketing | cod-rna    | cod-rna    | cod-rna    | covtype             | covtype             | covtype               | thyroid-ann | thyroid-ann | thyroid-ann       | thyroid-ann       |
| 0.90 0.80 0.79 | 0.75 0.71 0.70 | 1.03 0.91 0.89 | 0.95 0.88 0.86 | 0.86 0.80 0.71 | 0.69 0.62 0.60 | 0.94 0.80 0.78 | 0.91 0.78 0.76 | 0.80 0.68 0.67 | 0.66 0.58 0.57 | 0.89 0.76 0.75 | 0.86 0.74 0.72 |
| 0.86 0.80 0.77 | 0.74 0.69 0.68 | 1.01 0.88 0.87 | 0.94 0.86 0.84 | 1.98 1.64 1.58 | 1.46 1.23 1.22 | 2.39 1.90 1.82 | 2.36 1.83 1.81 | 6.73 4.77 4.69 | 4.42 3.08 3.19 | 8.03 5.86 5.59 | 8.39 5.69 5.95 |
| 0.82 0.71 0.71 | 0.69 0.62 0.60 | 0.94 0.80 0.78 | 0.91 0.78 0.76 | 0.70 0.60 0.60 | 0.57 0.50 0.50 | 0.77 0.64 0.64 | 0.72 0.58 0.60 | 0.60 0.53 0.52 | 0.50 0.42 0.44 | 0.68 0.57 0.59 | 0.65 0.55 0.53 |
| 0.80 0.68 0.67 | 0.66 0.58 0.57 | 0.89 0.76 0.75 | 0.85 0.74 0.72 | 3.22 2.42 2.37 | 2.11 1.46 1.51 | 3.27 2.77 2.21 | 3.55 2.54 2.59 | 0.80 0.68 0.66 | 0.65 0.57 0.56 | 0.88 0.76 0.75 | 0.85 0.74 0.72 |
| threads=2   | threads=3   | threads=4   | grid_choice=1 | grid_choice=2 | adaptivity_control=1 | adaptivity_control=2 | adaptivity_control=2, grid_choice=2 | voronoi=5 | voronoi=6 | voronoi=c(5,1000) | voronoi=c(6,1000) |
|             |             |             |               |                 |                      |                      |                                     |           |           |                   |                   |
| bank-marketing | bank-marketing | bank-marketing | cod-rna    | cod-rna    | covtype             | covtype             | covtype               | thyroid-ann | thyroid-ann | thyroid-ann       | thyroid-ann       |
| 3.27 2.93 2.88 | 2.76 2.57 2.53 | 3.94 3.40 3.33 | 3.43 3.02 2.97 | 2.59 2.24 2.16 | 2.05 1.86 1.81 | 2.60 2.54 2.54 | 2.66 2.30 2.27 | 2.38 1.94 1.87 | 1.80 1.65 1.65 | 2.30 1.82 1.81 |
| 2.59 2.24 2.16 | 2.05 1.86 1.81 | 2.60 2.54 2.54 | 2.66 2.30 2.27 | 2.38 1.94 1.87 | 1.80 1.65 1.65 | 2.30 1.82 1.81 | 2.37 1.99 1.92 | 2.22 1.80 1.73 | 1.65 1.43 1.40 | 2.30 1.82 1.81 |
| 2.38 1.94 1.87 | 1.80 1.65 1.65 | 2.30 1.82 1.81 | 2.37 1.99 1.92 | 2.22 1.80 1.73 | 1.65 1.43 1.40 | 2.30 1.82 1.81 | 2.37 1.99 1.92 | 6.25 4.79 4.59 | 3.96 3.12 3.01 | 8.52 6.17 5.88 |
| 6.25 4.79 4.59 | 3.96 3.12 3.01 | 8.52 6.17 5.88 | 7.39 5.19 4.91 | 26.62 17.29 16.50 | 14.26 9.80 9.44 | 34.18 22.27 21.72 | 34.64 23.01 21.19 | 1.89 1.55 1.56 | 1.39 1.24 1.21 | 2.40 1.92 1.88 |
| 1.89 1.55 1.56 | 1.39 1.24 1.21 | 2.40 1.92 1.88 | 2.37 1.99 1.92 | 1.69 1.31 1.31 | 1.23 1.09 1.07 | 2.16 1.68 1.64 | 1.49 1.16 1.19 | 10.08 8.04 7.40 | 5.35 4.59 3.96 | 12.53 7.97 7.92 |
| 10.08 8.04 7.40 | 5.35 4.59 3.96 | 12.53 7.97 7.92 | 9.49 6.62 6.97 | 1.69 1.31 1.31 | 1.23 1.09 1.07 | 2.16 1.68 1.64 | 1.49 1.16 1.19 | 2.20 1.77 1.73 | 1.66 1.43 1.41 | 2.73 2.17 2.08 |
| 2.20 1.77 1.73 | 1.66 1.43 1.41 | 2.73 2.17 2.08 | 2.23 1.84 1.76 | 2.21 1.81 1.76 | 1.65 1.43 1.41 | 2.75 2.17 2.12 | 2.22 1.80 1.73 | 1.81 1.54 1.54 | 1.59 1.57 1.67 | 2.12 1.81 1.77 |
| 1.81 1.54 1.54 | 1.59 1.57 1.67 | 2.12 1.81 1.77 | 2.02 1.72 1.69 | 2.21 1.81 1.76 | 1.65 1.43 1.41 | 2.75 2.17 2.12 | 2.22 1.80 1.73 | 1.40 1.27 1.22 | 1.17 1.10 1.05 | 1.66 1.41 1.39 |
| 1.40 1.27 1.22 | 1.17 1.10 1.05 | 1.66 1.41 1.39 | 1.38 1.22 1.17 | voronoi=c(5,1000) | voronoi=c(6,1000) | voronoi=c(5,1000) | voronoi=c(6,1000) | voronoi=c(5,1000) | voronoi=c(6,1000) | voronoi=c(5,1000) | voronoi=c(6,1000) |

Table 14: Training times (in sec.) for different compile architectures: from left to right they are SSE2, AVX, and AVX2, averaged over 10 repetitions with n=1000.

Table 15: Training times (in sec.) for different compile architectures: from left to right they are SSE2, AVX, and AVX2, averaged over 10 repetitions with n=2000.
Table 16: Training times (in sec.) for different compile architectures: from left to right they are SSE2, AVX, and AVX2, averaged over 10 repetitions with n=4000.

| threads=1 | threads=2 | threads=3 | grid_choice=1 | grid_choice=2 | adaptivity_control=1 | adaptivity_control=2 | adaptivity_control=2, grid_choice=2 | voronoi=c(5,1000) | voronoi=c(6,1000) |
|-----------|-----------|-----------|---------------|---------------|----------------------|----------------------|-----------------------------------|-------------------|------------------|
| threads=1 | 12.55     | 11.34     | 11.10         | 10.51         | 9.85                 | 9.71                 | 15.41               | 13.35             | 12.99            |
| threads=2 | 9.12      | 7.80      | 7.55          | 7.01          | 6.35                 | 6.11                 | 11.60               | 9.52              | 9.21             |
| threads=3 | 8.29      | 6.78      | 6.64          | 6.10          | 5.36                 | 5.28                 | 10.68               | 8.47              | 8.19             |
| threads=4 | 7.98      | 6.44      | 6.31          | 5.78          | 4.99                 | 4.88                 | 10.43               | 8.10              | 7.76             |
| grid_choice=1 | 25.30 | 17.98    | 17.32         | 14.10         | 10.86                | 10.38                | 34.80               | 24.00             | 23.43           |
| grid_choice=2 | 112.65 | 73.27   | 70.09         | 52.64         | 36.40                | 35.28                | 152.60              | 100.76            | 96.10           |
| adaptivity_control=1 | 6.82    | 5.73    | 5.52          | 4.96          | 4.28                | 4.37                | 9.18                | 7.34              | 6.90             |
| adaptivity_control=2 | 5.59    | 4.82    | 4.61          | 4.15          | 3.95                | 3.66                | 8.44                | 6.30              | 6.14             |
| adaptivity_control=2, grid_choice=2 | 38.92   | 28.29   | 27.22         | 18.85         | 14.05                | 13.02                | 46.64               | 24.79             | 26.79            |
| voronoi=5 | 5.33      | 4.35      | 4.45          | 4.54          | 4.62                | 4.37                | 7.34                | 5.32              | 5.71             |
| voronoi=6 | 3.60      | 2.96      | 2.86          | 2.84          | 2.53                | 2.44                | 4.88                | 3.92              | 3.78             |
| voronoi=c(5,1000) | 4.88    | 4.18    | 4.15          | 4.22          | 3.83                | 3.60                | 5.35                | 4.11              | 4.10            |
| voronoi=c(6,1000) | 2.72    | 2.36    | 2.38          | 2.31          | 2.09                | 2.15                | 3.25                | 2.76              | 2.73             |

Table 17: Training times (in sec.) for different compile architectures: from left to right they are SSE2, AVX, and AVX2, averaged over 10 repetitions with n=6000.

| threads=1 | threads=2 | threads=3 | grid_choice=1 | grid_choice=2 | adaptivity_control=1 | adaptivity_control=2 | adaptivity_control=2, grid_choice=2 | voronoi=c(5,1000) | voronoi=c(6,1000) |
|-----------|-----------|-----------|---------------|---------------|----------------------|----------------------|-----------------------------------|-------------------|------------------|
| threads=1 | 27.87     | 25.27     | 24.72         | 23.10         | 21.83                | 21.44                | 33.86               | 29.46             | 28.85           |
| threads=2 | 19.69     | 16.91     | 16.48         | 14.93         | 13.52                | 13.30                | 24.96               | 20.53             | 19.93           |
| threads=3 | 17.89     | 14.89     | 14.67         | 13.21         | 11.65                | 11.48                | 23.09               | 18.42             | 17.90           |
| threads=4 | 17.35     | 14.06     | 13.81         | 12.52         | 10.80                | 10.64                | 22.46               | 17.52             | 16.99           |
| grid_choice=1 | 57.15    | 41.01    | 39.40         | 30.85         | 23.84                | 23.25                | 79.98               | 55.21             | 53.80           |
| grid_choice=2 | 266.36  | 176.77   | 168.54        | 121.97        | 82.49                | 79.26                | 376.11              | 241.72            | 234.04          |
| adaptivity_control=1 | 14.67   | 12.41    | 12.11         | 10.95         | 9.64                 | 9.69                 | 19.78               | 14.99             | 14.71           |
| adaptivity_control=2 | 11.55   | 10.27    | 10.32         | 9.16          | 8.48                 | 8.31                 | 16.68               | 13.53             | 13.37           |
| adaptivity_control=2, grid_choice=2 | 91.60   | 58.95    | 58.69         | 36.09         | 28.60                | 27.50                | 65.50               | 50.19             | 47.58           |
| voronoi=5 | 9.26      | 7.80      | 7.56          | 7.27          | 7.03                | 6.39                 | 13.32               | 9.16              | 8.78            |
| voronoi=6 | 5.27      | 4.47      | 4.46          | 4.17          | 3.66                | 3.64                 | 6.74                | 5.47              | 5.29            |
| voronoi=c(5,1000) | 8.27    | 6.82    | 6.71          | 7.88          | 6.23                | 6.89                 | 9.70                | 8.47              | 8.56            |
| voronoi=c(6,1000) | 3.84    | 3.61    | 3.61          | 3.34          | 2.98                | 2.97                 | 4.57                | 4.19              | 4.19            |