Tutorial to GURLS usage for recursive RLS

Introduction 1

Recursive RLS is an efficient algorithm for efficient update of the exact RLS estimator when the data are given sequentially as in online learning, as for any new input-output pair the (regularized) inverse of the kernel matric in the primal space is updated just via matrix/vector multiplication. The basic operations of recursive RLS are sketched in Algorithm 1.1.

```
Algorithm 1.1 Recursive RLS
```

```
given:
      the initial RLS estimator \boldsymbol{w}_{\boldsymbol{n}_0}
      the inverse of the (regularized) kernel matrix, \mathbf{C}_{n_0}^{-1}
      an order sequence of input-output pairs \{(x_{n_0+1},y_{n_0+1}),\ldots,(x_{n_{\max}},y_{n_{\max}})\}
for \ \mathbf{n}=\mathbf{n_0},...,\mathbf{n_{max}}-1 \ do
                                      \mathbf{w_{n+1}} = \mathbf{w_n} + \frac{\mathbf{C_n^{-1}}}{1 + \mathbf{x_n^T C_n^{-1} x_n}} \mathbf{x_n} (\mathbf{y_n} - \mathbf{x_n^T w_n})
end for
return \ w_{n_{\max}}
```

Design

Recursive RLS can be performed in GURLS (GURLS⁺⁺) through the tasks (subclasses in GURLS⁺⁺) primalrecinit and primalrecupdate of the category (class in GURLS⁺⁺) rls. The workflow for rank 1 update of the RLS estimator in GURLS and GURLS⁺⁺ is depicted in Figure 2. Initial parameter selection and training are carried out on a initial set of samples. The computation of the RLS estimator is carried out by the task primalrecinit of the category rls, which stores all information necessary for efficient recursive update in the options structure. Once the information about initial training is stored in the options' structure, opt, given a new set of input-output pairs (possibly also just one pair), the RLS estimator can be efficiently updated via the task primalrecupdate of the category rls. Every time a new set of inputoutput pairs is available, task primalrecupdate can be invoked again. Parameter selection and RLS estimation (Retraining in Figure 2) can be repeated after any number of online updates. Finally, the ordinary task primal of the prediction category can be used on test data.

Rank 1 update of the RLS estimator is thus efficiently implemented in GURLS thanks to the two new tasks of the category rls, primalrecinit, and primalrecupdate. As all GURLS tasks, primalrecinit and primalrecupdate take in input:

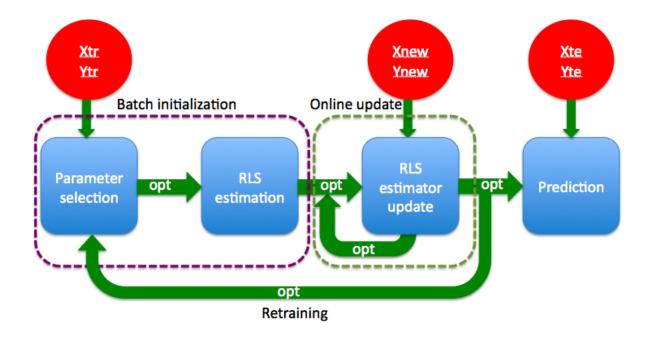


Figure 1: Representation of GURLS design for RLS via recursive rank 1 update or the RLS estimator

- an input data matrix
- a labels matrix
- an options' structure

and return just one output variable, which is a structure containing the fields

- W: matrix of coefficient vectors of rls estimator for each class
- C: empty matrix
- X: empty matrix
- XtX: the kernel matrix in the primal space
- Cinv: inverse of the regularized kernel matrix in the primal space

Task primalrecinit is indeed almost identical to task primal of the rls category, which implements the RLS estimator for batch learning. The only difference is in the last two fields of the output structure, XtX and Cinv, which are not returned by task primal of the rls category.

2.1 GURLS **usage**

An example of GURLS usage for rank 1 update of the RLS estimator can be found in the demo demo_recursiveRLS.m in the demo directory. The demo is structured in four steps, of which the salient part are reported in the following:

1. Initial parameter selection and training

```
name = 'ExampleExperiment';
opt = defopt(name);
opt.kernel.XtX = Xtr'*Xtr;
opt.kernel.Xty = Xtr'*ytr;
opt.kernel.n = size(ytr,1);
opt.seq = {'split:ho','paramsel:hoprimal','rls:primalrecinit'};
opt.process{1} = [2,2,2];
opt = gurls (Xtr, ytr, opt,1);
```

Notice that while parameter selection can be carried out via any of the tasks for batch parameter selection available in Gurls and Gurls⁺⁺, for initial estimation of the RLS estimator the specific task primalrecinit has to be invoked.

2. Online update, to be repeated every time a new set of input-output pairs is available

```
opt.rls = rls_primalrecupdate(Xnew, ynew, opt);
opt.kernel.XtX = opt.kernel.XtX + Xnew'*Xnew;
opt.kernel.Xty = opt.kernel.Xty + Xnew'*ynew;
opt.kernel.n = opt.kernel.n + size(ynew,1);
```

3. Prediction

```
ypred = pred_primal(Xte, yte, opt);
```

4. Retraining

```
optRetrained = defopt(name);
optRetrained.kernel = opt.kernel;
optRetrained.split.tr = zeros(opt.kernel.n,1);
optRetrained.split.va = 1:size(yva,1);
optRetrained.seq = {'paramsel:hoprimal','rls:primalrecinit','pred:primal','per
optRetrained.process{1} = [2,2,0,0];
optRetrained.process{2} = [3,3,2,2];
optRetrained = gurls (Xva, yva, optRetrained,1);
optRetrained = gurls (Xte, yte, optRetrained,2);
```

Notice that selection of the new regularization parameter is performed via hold-out validation using a subset Xva, yva of the total training set as validation set.

2.2 GURLS⁺⁺usage

As for GURLS, recursive RLS can be performed in GURLS⁺⁺ using the the same pipelines and tasks described in Subsection 2.1. The GURLS tasks primalrecinit and primalrecupdate of the category rls have been implemented in GURLS⁺⁺ as subclasses of the class rls.

However, in order to simplify GURLS⁺⁺usage for recursive RLS, we are working on implementing a specific class, namely RecursiveRLS, which methods Train, Update, Retrain, Prediction shall be user friendly wrappers to the set of pipelines and tasks that implement the 4 steps i) batch initialization, ii) online update iii) prediction iv) retraining, as shown in Figure 2.2.

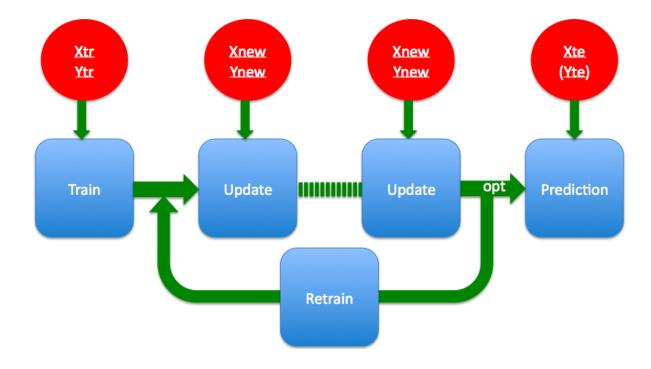


Figure 2: Representation of GURLS⁺⁺ design for RLS via recursive rank 1 update or the RLS estimator

3 Experiments

We have used the GURLS implementation of the rank 1 update of the RLS estimator on the bio data set used in [1], which is stored into four files:

- 'Xtrain.csv': containing the training input $n \times d$ data matrix, where n is the number of samples (12,471) and d is the number of variables (68)
- 'Ytrain.csv': containing the input $n \times 1$ label vector
- 'Xtest.csv': containing the test input $n_{test} \times d$ data matrix, with $n_{test} = 12,471$.
- 'Ytest.csv': containing the input $n_{test} \times 1$ label vector

We used the first n_0 samples of the training data for initial parameter selection and training. Recursive rank 1 update of the RLS estimator is performed on the remaining training samples. Online learning behavior is simulated by reading blocks of new samples from the files 'Xtrain.csv' and 'Ytrain.csv', and sequentially invoking task rls:primalrecupdate on each set of samples, until all lines of the files have been read. Online learning is performed for increasing value of n_0 , precisely from 10 to 200 increasing of 10 samples each time. On the same data set, batch learning is performed by training an RLS estimator from the entire training set in batch mode, using the same parameter selected in the initial parameter selection of online RLS. The experiment is repeated 10 times, each time after random permutation of the training set samples. We evaluated the mean difference between accuracies of online and batch RLS, and the mean frobenius norm of the difference of the test labels predicted by the two methods. While accuracies are identical, the values of the the predicted test labels (before class assignment) are slightly different the difference between the estimated test labels, though already

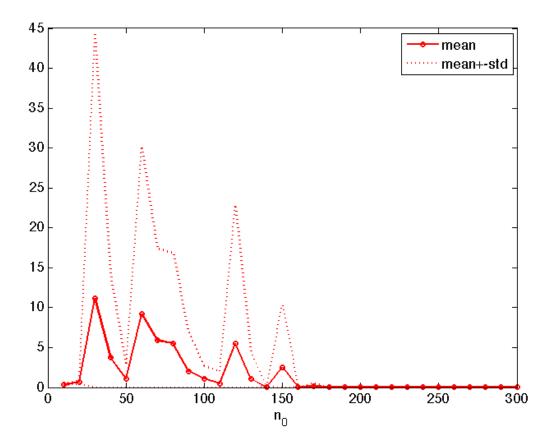


Figure 3: Frobenius norm of the difference between test labels predicted by online and batch RLS estimators.

very small for small n_0 , decreases with n_0 , and stabilizes for n_0 is significantly bigger than the number of features, 68. Such a slight difference may be due to the, when $n_0 < d$ inversion of the kernel matrix in the primal space may lead to some instability.

Bibliography

[1] F. Lauer and Y. Guermeur. Msvmpack: A multi-class support vector machine package. *The Journal of Machine Learning Research*, 12:2293–2296, 2011.