APA-L6

September 6, 2018

1 APA Laboratori 6 - MLP and the RBF

```
In [1]: # uncomment to install missing libraries
        # install.packages('nnet')
        # install.packages('caret')
        # install.packages('cclust')
```

```
In [2]: options(repr.plot.width=6, repr.plot.height=6)
```

```
In [3]: library(MASS)
        library(nnet)
        set.seed (4567)
```

1.1 Multilayer Perceptron Example 1: Admission into graduate school data

Suppose we are interested in how variables, such as
GRE (Graduate Record Exam scores)
GPA (Grade Point Average) and
rank (prestige of the undergraduate institution)
affect admission into a graduate school.

The target variable, admit/don't admit, is a binary variable, which we want to characterize and, if possible, to predict (a model)

```
In [4]: Admis <- read.csv("Admissions.csv")
```

view the first few rows of the data

```
In [5]: head(Admis)
```

admit	gre	gpa	rank
0	380	3.61	3
1	660	3.67	3
1	800	4.00	1
1	640	3.19	4
0	520	2.93	4
1	760	3.00	2

We will treat all the variables gre and gpa as continuous.

The variable rank takes on the values 1 through 4, so we can fairly treat it as numerical (although, in rigour, it is ordinal)

```
In [6]: Admis$admit <- factor(Admis$admit, labels=c("No","Yes"))

        summary(Admis)

        N <- nrow(Admis)
```

```
 admit          gre             gpa             rank
 No :273   Min.   :220.0   Min.   :2.260   Min.   :1.000
 Yes:127   1st Qu.:520.0   1st Qu.:3.130   1st Qu.:2.000
           Median :580.0   Median :3.395   Median :2.000
           Mean   :587.7   Mean   :3.390   Mean   :2.485
           3rd Qu.:660.0   3rd Qu.:3.670   3rd Qu.:3.000
           Max.   :800.0   Max.   :4.000   Max.   :4.000
```

We first split the available data into learning and test sets, selecting randomly 2/3 and 1/3 of the data We do this for a honest estimation of prediction performance

```
In [7]: set.seed(43)

        learn <- sample(1:N, round(2*N/3))

        nlearn <- length(learn)
        ntest <- N - nlearn
```

We start using logistic regression (a linear classifier)

```
In [8]: model.logreg <- glm (admit~., data=Admis[learn,], family=binomial)

        summary(model.logreg)
```

```
Call:
glm(formula = admit ~ ., family = binomial, data = Admis[learn,
    ])

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.6190  -0.9154  -0.6441   1.1249   2.1551

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -3.879084   1.403346  -2.764 0.005707 **
gre          0.001468   0.001307   1.124 0.261161
gpa          1.074822   0.396957   2.708 0.006776 **
rank        -0.566394   0.152750  -3.708 0.000209 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

```
(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 341.27  on 266  degrees of freedom
Residual deviance: 312.22  on 263  degrees of freedom
AIC: 320.22

Number of Fisher Scoring iterations: 3
```

Simplify the model using the AIC

```
In [9]: model.logreg2 <- step(model.logreg)

Start:  AIC=320.22
admit ~ gre + gpa + rank

       Df Deviance    AIC
- gre   1   313.49 319.49
<none>      312.22 320.22
- gpa   1   319.91 325.91
- rank  1   327.04 333.04

Step:  AIC=319.49
admit ~ gpa + rank

       Df Deviance    AIC
<none>      313.49 319.49
- gpa   1   324.69 328.69
- rank  1   329.40 333.40
```

The new model has one variable less and the error (residual deviance) is virtually the same (313.5 vs 312.2)

Interpretation of the coefficients

```
In [10]: exp(model.logreg2$coefficients)
```

(Intercept) 0.0315371431069108 **gpa** 3.38896809056484 **rank** 0.559018874202768

Calculation of apparent error in the training set (learn)

```
In [11]: glfpred=NULL
         glfpred[model.logreg2$fitted.values<0.5]=0
         glfpred[model.logreg2$fitted.values>=0.5]=1
         table(Admis$admit[learn],glfpred)
         error_rate.learn <- 100*(1-sum(diag(table(Admis$admit[learn],glfpred)))/nlearn)
         error_rate.learn
```

```
     glfpred
        0   1
  No  163  14
  Yes  63  27
```

28.8389513108614
we get a learning error which is quite high (28.84%)
Estimation of prediction error using the test set

```
In [12]: glft = predict(model.logreg2, newdata=Admis[-learn,])
         pt = 1/(1+exp(-glft))
         glfpredt = NULL
         glfpredt[pt<0.5]=0
         glfpredt[pt>=0.5]=1
         table(Admis$admit[-learn],glfpredt)
         error_rate.test <- 100*(1-sum(diag(table(Admis$admit[-learn],glfpredt)))/ntest)
         error_rate.test
```

```
     glfpredt
       0  1
  No  87  9
  Yes 27 10
```

27.0676691729323
we get a prediction error of 27.07%
Now we switch to non-linear modelling with a MLP
The nnet() function is quite powerful and very reliable from the optimization point fo view. From the computational point of view, it has two drawbacks:

1. it does not have a built-in mechanism for multiple runs or cross-validation
2. it only admits networks of one hidden layer (of size 'size')

Please have a look at nnet before going any further

```
In [13]: ?nnet
```

The basic parameters are 'size' and 'decay' (the regularization constant, lambda) As usual, R detects it is a classification problem because 'admit' is a factor It buils a MLP with one output neuron (just two classes), with the logistic function and uses the cross-entropy as error function
Let's start by scaling of inputs, this is important to avoid network 'stagnation' (premature convergence)

```
In [14]: Admis$gpa <- scale(Admis$gpa)
         Admis$gre <- scale(Admis$gre)
         Admis$rank <- scale(Admis$rank)
         head(Admis)
```

admit	gre	gpa	rank
No	-1.7980110	0.5783479	0.5452850
Yes	0.6258844	0.7360075	0.5452850
Yes	1.8378321	1.6031352	-1.5723268
Yes	0.4527490	-0.5252692	1.6040909
No	-0.5860633	-1.2084607	1.6040909
Yes	1.4915613	-1.0245245	-0.5135209

To illustrate the first results, we just fit a MLP with 2 hidden neurons

```
In [15]: model.nnet <- nnet(admit ~., data = Admis, subset=learn, size=2, maxit=200, decay=0)

# weights:  11
initial  value 185.455554
iter  10 value 154.303985
iter  20 value 151.180313
iter  30 value 151.033446
iter  40 value 150.080157
iter  50 value 149.658535
iter  60 value 149.551399
iter  70 value 149.170569
iter  80 value 149.010636
iter  90 value 148.893029
iter 100 value 148.692015
iter 110 value 148.663268
final  value 148.662975
converged
```

Take your time to understand the output

```
In [16]: model.nnet

a 3-2-1 network with 11 weights
inputs: gre gpa rank
output(s): admit
options were - entropy fitting
```

In particular, understand why the total number of weights is 11, what 'initial value' and 'final value' are and what does 'converged' mean

This is the final value of the error function (also known as fitting criterion)

```
In [17]: model.nnet$value
```

148.66297495079

fitted values for the training data

```
In [18]: model.nnet$fitted.values
```

195	0.35185339
364	0.38732833
23	0.29440536
281	0.48609440
125	0.31717859
215	0.37013893
268	0.31226305
200	0.29968619
72	0.04476478
342	0.29523687
153	0.50237884
62	0.29569985
253	0.68539131
102	0.31006383
184	0.52436669
258	0.33656979
95	0.33549133
81	0.29435951
11	0.29874178
44	0.30422394
367	0.04527828
332	0.30645052
64	0.31883737
4	0.29489290
137	0.29574790
59	0.10881562
324	0.04685942
214	0.30127777
266	0.04820393
390	0.34957475
289	0.29447091
34	0.31813217
140	0.71413461
52	0.04478516
300	0.29966028
379	0.29743140
255	0.29552323
208	0.71082617
36	0.05224385
182	0.30469275
18	0.04487824
307	0.45587175
366	0.04495515
50	0.04802087
33	0.30301266
30	0.54706116
5	0.04475784
288	0.29741840
104	0.35100246
354	0.33898154
143	0.30198744
171	0.05025795

and the residuals

```
In [19]: model.nnet$residuals
```

195	0.64814661
364	-0.38732833
23	-0.29440536
281	-0.48609440
125	-0.31717859
215	0.62986107
268	0.68773695
200	-0.29968619
72	-0.04476478
342	0.70476313
153	0.49762116
62	-0.29569985
253	0.31460869
102	-0.31006383
184	0.47563331
258	0.66343021
95	0.66450867
81	-0.29435951
11	-0.29874178
44	-0.30422394
367	-0.04527828
332	-0.30645052
64	0.68116263
4	0.70510710
137	-0.29574790
59	-0.10881562
324	-0.04685942
214	-0.30127777
266	-0.04820393
390	-0.34957475
289	-0.29447091
34	0.68186783
140	0.28586539
52	-0.04478516
300	-0.29966028
379	-0.29743140
255	0.70447677
208	0.28917383
36	-0.05224385
182	-0.30469275
18	-0.04487824
307	0.54412825
366	-0.04495515
50	-0.04802087
33	-0.30301266
30	-0.54706116
5	-0.04475784
288	0.70258160
104	-0.35100246
354	-0.33898154
143	-0.30198744
171	-0.05025795

Now look at the weights

```
In [20]: model.nnet$wts
```

1. -144.914377636294 2. -115.574875427068 3. -29.5397472905414 4. 29.8620638100509 5. 6.04841812135005 6. 0.450634574495237 7. -1.11572636677264 8. 1.53595357722862 9. 41.6437693062623 10. -2.19154009113553 11. -42.5193847645286

I think this way is clearer:

```
In [21]: summary(model.nnet)
```

```
a 3-2-1 network with 11 weights
options were - entropy fitting
  b->h1  i1->h1  i2->h1  i3->h1
-144.91 -115.57  -29.54   29.86
  b->h2  i1->h2  i2->h2  i3->h2
   6.05    0.45   -1.12    1.54
   b->o   h1->o   h2->o
  41.64   -2.19  -42.52
```

i1,i2,i3 are the 3 inputs, h1, h2 are the two hidden neurons, b is the bias (offset)

As you can see, some weights are large (two orders of magnitude larger then others) This is no good, since it makes the model unstable (i.e., small changes in some inputs may entail significant changes in the network, because of the large weights)

One way to avoid this is by regularizing the learning process:

```
In [22]: model.nnet <- nnet(admit ~., data = Admis,
                            subset=learn, size=2, maxit=200, decay=0.01)
```

```
# weights:  11
initial  value 212.163281
iter  10 value 156.961946
iter  20 value 153.125715
iter  30 value 152.156794
iter  40 value 152.087114
iter  50 value 152.086597
final  value 152.086580
converged
```

notice the big difference

```
In [23]: model.nnet$wts

         summary(model.nnet)
```

1. 6.53419063936293 2. 0.543714592171317 3. -2.74234950830059 4. 3.39359863471471 5. -3.36715081295151 6. -1.18039931310529 7. -0.709407171560226 8. 0.829696661234554 9. 2.51020989996937 10. -3.14715629970143 11. -4.16929761475168

```
a 3-2-1 network with 11 weights
options were - entropy fitting  decay=0.01
 b->h1 i1->h1 i2->h1 i3->h1
  6.53   0.54  -2.74   3.39
 b->h2 i1->h2 i2->h2 i3->h2
 -3.37  -1.18  -0.71   0.83
 b->o h1->o h2->o
 2.51 -3.15 -4.17
```

Now let's compute the training error

```
In [24]: p1 <- as.factor(predict (model.nnet, type="class"))

         t1 <- table(p1,Admis$admit[learn])
         error_rate.learn <- 100*(1-sum(diag(t1))/nlearn)
         error_rate.learn
```

28.0898876404494

And the corresponding test error

```
In [25]: p2 <- as.factor(predict (model.nnet, newdata=Admis[-learn,], type="class"))

         t2 <- table(p2,Admis$admit[-learn])
         error_rate.test <- 100*(1-sum(diag(t2))/ntest)
         error_rate.test
```

26.3157894736842

We get 26.32%, so it seems that the MLP helps a little bit; however, we need to work harder

We are going to do the modelling in a principled way now. Using 10x10 CV to select the best combination of 'size' and 'decay'

Just by curiosity, let me show you that we can fit any dataset (in the sense of reducing the training error):

```
In [26]: model.nnet <- nnet(admit ~., data = Admis,
                            subset=learn, size=20, maxit=200, trace=T)

# weights:  101
initial  value 201.805819
iter  10 value 153.848554
iter  20 value 138.333699
iter  30 value 126.583519
iter  40 value 118.200209
iter  50 value 106.232510
iter  60 value 94.855899
iter  70 value 81.443226
iter  80 value 72.072775
iter  90 value 66.247734
iter 100 value 63.543149
```

```
iter 110 value 60.713822
iter 120 value 57.034778
iter 130 value 55.760224
iter 140 value 54.653371
iter 150 value 53.141961
iter 160 value 51.878818
iter 170 value 50.818868
iter 180 value 48.734692
iter 190 value 47.855112
iter 200 value 47.016154
final  value 47.016154
stopped after 200 iterations
```

Now let's compute the training error

```
In [27]: p1 <- as.factor(predict (model.nnet, type="class"))

         (t1 <- table(p1,Admis$admit[learn]))
         error_rate.learn <- 100*(1-sum(diag(t1))/nlearn)
         error_rate.learn
```

```
p1     No Yes
  No  172  12
  Yes   5  78
```

6.36704119850188

And the corresponding test error

```
In [28]: p2 <- as.factor(predict (model.nnet,
                                  newdata=Admis[-learn,], type="class"))

         (t2 <- table(p2,Admis$admit[-learn]))
         error_rate.test <- 100*(1-sum(diag(t2))/ntest)
         error_rate.test
```

```
p2    No Yes
  No  66  23
  Yes 30  14
```

39.8496240601504

That's it: we got a training error around 6% (four times lower than the previous one), but it is illusory ... the test error is larger than before (around 40%); The relevant comparison is between 6% and 40%, this large gap is an indication of overfitting

{caret} is an excellent package for training control, once you know what all these concepts are

WARNING: if the package is not installed in your computer, installation needs some previous packages

```
In [29]: library(caret)
```

```
Loading required package: lattice
Loading required package: ggplot2
```

For a specific model, in our case the neural network, the function train() in {caret} uses a "grid" of model parameters and trains using a given resampling method (in our case we will be using 10x10 CV). All combinations are evaluated, and the best one (according to 10x10 CV) is chosen and used to construct a final model, which is refit using the whole training set

Thus train() returns the constructed model (exactly as a direct call to nnet() would)

In order to find the best network architecture, we are going to explore two methods:

1. Explore different numbers of hidden units in one hidden layer, with no regularization
2. Fix a large number of hidden units in one hidden layer, and explore different regularization values (recommended)

doing both (explore different numbers of hidden units AND regularization values) is usually a waste of computing resources (but notice that train() would admit it)

Let's start with 1.

set desired sizes

```
In [30]: (sizes <- 2*seq(1,10,by=1))
```

1. 2 2. 4 3. 6 4. 8 5. 10 6. 12 7. 14 8. 16 9. 18 10. 20

specify 10x10 CV

```
In [31]: trc <- trainControl (method="repeatedcv", number=10, repeats=10)
```

```
model.10x10CV <- train (admit ~.,
                        data = Admis,
                        subset=learn,
                        method='nnet',
                        maxit = 500,
                        trace = FALSE,
                        tuneGrid = expand.grid(.size=sizes,.decay=0),
                        trControl=trc)
```

We can inspect the full results

```
In [32]: model.10x10CV$results
```

size	decay	Accuracy	Kappa	AccuracySD	KappaSD
2	0	0.6794302	0.15838888	0.06555800	0.1590611
4	0	0.6528063	0.12692082	0.07015772	0.1571809
6	0	0.6364245	0.10645660	0.08609798	0.1904523
8	0	0.6242023	0.10665279	0.07449450	0.1566918
10	0	0.6084473	0.09292062	0.08412655	0.1810415
12	0	0.6200997	0.12755055	0.08120269	0.1805066
14	0	0.6071368	0.10486461	0.08483468	0.1816216
16	0	0.6048291	0.10629726	0.09154840	0.1882389
18	0	0.6144160	0.13036946	0.09400006	0.1935479
20	0	0.6032906	0.11403299	0.07941761	0.1685627

and the best model found

```
In [33]: model.10x10CV$bestTune
```

size	decay
2	0

The results are quite disappointing ...
Now method 2.

```
In [34]: (decays <- 10^seq(-3,0,by=0.1))
```

1. 0.001 2. 0.00125892541179417 3. 0.00158489319246111 4. 0.00199526231496888 5. 0.00251188643150958 6. 0.00316227766016838 7. 0.00398107170553497 8. 0.00501187233627272 9. 0.00630957344480193 10. 0.00794328234724281 11. 0.01 12. 0.0125892541179417 13. 0.0158489319246111 14. 0.0199526231496888 15. 0.0251188643150958 16. 0.0316227766016838 17. 0.0398107170553497 18. 0.0501187233627272 19. 0.0630957344480193 20. 0.0794328234724282 21. 0.1 22. 0.125892541179417 23. 0.158489319246111 24. 0.199526231496888 25. 0.251188643150958 26. 0.316227766016838 27. 0.398107170553497 28. 0.501187233627272 29. 0.630957344480194 30. 0.794328234724282 31. 1

WARNING: this takes a few minutes

```
In [35]: model.10x10CV <- train (admit ~.,
                                  data = Admis,
                                  subset=learn,
                                  method='nnet',
                                  maxit = 500,
                                  trace = FALSE,
                                  tuneGrid = expand.grid(.size=20,.decay=decays),
                                  trControl=trc)
```

We can inspect the full results

```
In [36]: model.10x10CV$results
```

size	decay	Accuracy	Kappa	AccuracySD	KappaSD
20	0.001000000	0.6107835	0.1259526	0.09998091	0.2119052
20	0.001258925	0.6013960	0.1134127	0.09339224	0.1969092
20	0.001584893	0.6080484	0.1263137	0.10416937	0.2231088
20	0.001995262	0.6066952	0.1225178	0.09008144	0.1928053
20	0.002511886	0.6099573	0.1153077	0.09470323	0.2109673
20	0.003162278	0.6134473	0.1333902	0.08670615	0.1955272
20	0.003981072	0.6054701	0.1080233	0.08168971	0.1821464
20	0.005011872	0.6167094	0.1306518	0.09054663	0.2045439
20	0.006309573	0.6198291	0.1394422	0.09137005	0.2030928
20	0.007943282	0.6174786	0.1337744	0.08856300	0.1877713
20	0.010000000	0.6229202	0.1382363	0.08509643	0.1941121
20	0.012589254	0.6337179	0.1558897	0.08952936	0.1982104
20	0.015848932	0.6337464	0.1445271	0.07706627	0.1737916
20	0.019952623	0.6423504	0.1560546	0.08046036	0.1868632
20	0.025118864	0.6452137	0.1584320	0.08295725	0.1906374
20	0.031622777	0.6485613	0.1620090	0.09131440	0.2108199
20	0.039810717	0.6466667	0.1419667	0.07964091	0.1829152
20	0.050118723	0.6482764	0.1327201	0.07951758	0.1845405
20	0.063095734	0.6527208	0.1368859	0.07962402	0.1852097
20	0.079432823	0.6625071	0.1467353	0.07182677	0.1759579
20	0.100000000	0.6778632	0.1772463	0.07263787	0.1820088
20	0.125892541	0.6835328	0.1818679	0.07305955	0.1887729
20	0.158489319	0.6879772	0.1916028	0.06630907	0.1715492
20	0.199526231	0.6920798	0.1992488	0.06563574	0.1692387
20	0.251188643	0.6983903	0.2154530	0.06596567	0.1743141
20	0.316227766	0.6987607	0.2100540	0.06268639	0.1680927
20	0.398107171	0.6987749	0.2074932	0.06240388	0.1702630
20	0.501187234	0.6980484	0.2026805	0.05877363	0.1616328
20	0.630957344	0.6991738	0.2006121	0.05839574	0.1638297
20	0.794328235	0.6969231	0.1891162	0.05786888	0.1619998
20	1.000000000	0.6920513	0.1685243	0.05420725	0.1507764

and the best model found

```
In [37]: model.10x10CV$bestTune
```

```
save(model.10x10CV, file = "model.10x10CV.regul")
```

```
load ("model.10x10CV.regul")
```

	size	decay
29	20	0.6309573

The results are a bit better; we should choose the model with the lowest 10x10CV error overall, in this case it corresponds to 20 hidden neurons, with a decay of 0.3162278

So what remains is to predict the test set with our final model

```
In [38]: p2 <- as.factor(predict (model.10x10CV,
                                  newdata=Admis[-learn,], type="raw"))
```

```
t2 <- table(pred=p2,truth=Admis$admit[-learn])
error_rate.test <- 100*(1-sum(diag(t2))/ntest)
error_rate.test
```

27.8195488721805

We get 27.82% after all this work; it seems that the information in this dataset is not enough to accurately predict admittance. Note that ...

... upon looking at the confusion matrix for the predictions ...

```
In [39]: t2
```

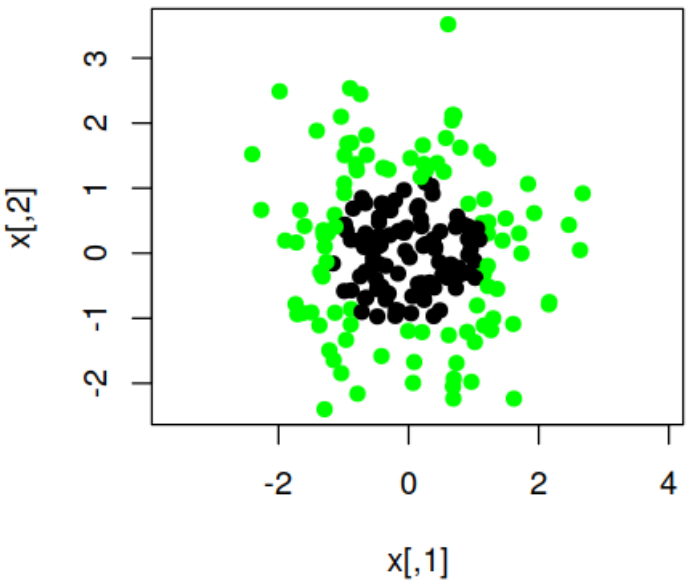
```
     truth
pred  No Yes
  No  87  28
  Yes  9   9
```

it clearly suggests that quite a lot of people is getting accepted when they should not, given their gre, gpa and rank It is very likely that other (subjective?) factors are being taken into account, that are not in the dataset

---

1.2 Multilayer Perceptron Example 2: circular artificial 2D data

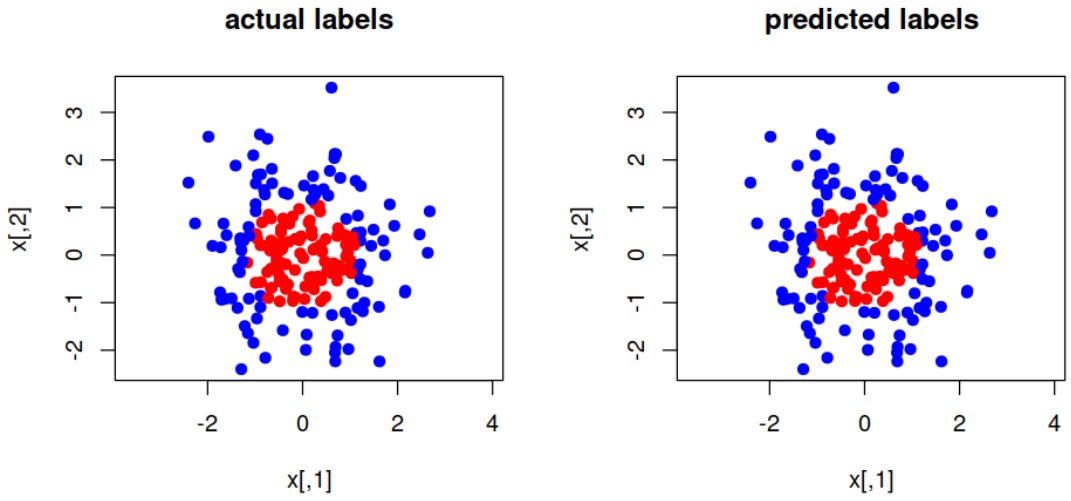
```
In [40]: options(repr.plot.width=4, repr.plot.height=4)

         set.seed(3)

         p <- 2
         N <- 200

         x <- matrix(rnorm(N*p),ncol=p)
         y <- as.numeric((x[,1]^2+x[,2]^2) > 1.4)
         mydata <- data.frame(x=x,y=y)
         plot(x,col=c('black','green')[y+1],pch=19,asp=1)
```



Let's use one hidden layer, 3 hidden units, no regularization and the error function "cross-entropy" In this case it is not necessary to standardize because they variables already are (they have been generated from a distribution with mean 0 and standard deviation 1).

```
In [41]: nn1 <- nnet(y~x.1+x.2,
                     data=mydata,
                     entropy=T,
                     size=3,
                     decay=0,
                     maxit=2000,
                     trace=F)

         yhat <- as.numeric(predict(nn1,type='class'))
```

```
In [42]: options(repr.plot.width=8, repr.plot.height=4)
         par(mfrow=c(1,2))
         plot(x,
              pch=19,
              col=c('red','blue')[y+1],
              main='actual labels',asp=1)
         plot(x,col=c('red','blue')[(yhat>0.5)+1],
              pch=19,
              main='predicted labels',
              asp=1)
```




```
In [43]: table(actual=y,predicted=predict(nn1,type='class'))
```

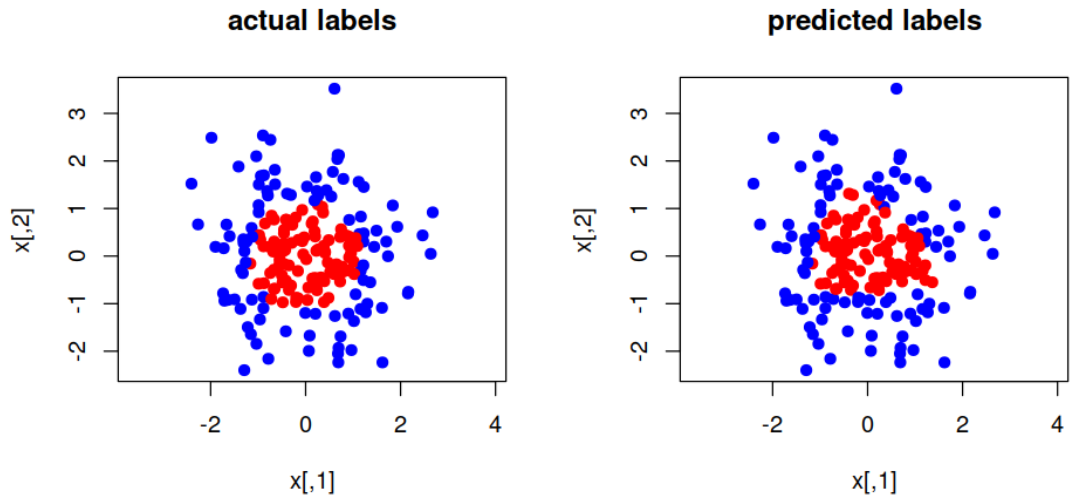
```
      predicted
actual   0   1
     0 100   0
     1   0 100
```

Excellent, indeed

Let's execute it again, this time wth a different random seed

```
In [44]: options(repr.plot.width=8, repr.plot.height=4)
         set.seed(4)

         nn1 <- nnet(y~x.1+x.2,
                     data=mydata,
                     entropy=T,
                     size=3,
                     decay=0,
                     maxit=2000,
                     trace=F)
         yhat <- as.numeric(predict(nn1,type='class'))
         par(mfrow=c(1,2))
         plot(x,
              pch=19,
              col=c('red','blue')[y+1],
              main='actual labels',asp=1)
         plot(x,
              col=c('red','blue')[(yhat>0.5)+1],
```

```
       pch=19,
       main='predicted labels',asp=1)
```




```
In [45]: table(actual=y,predicted=predict(nn1,type='class'))
```

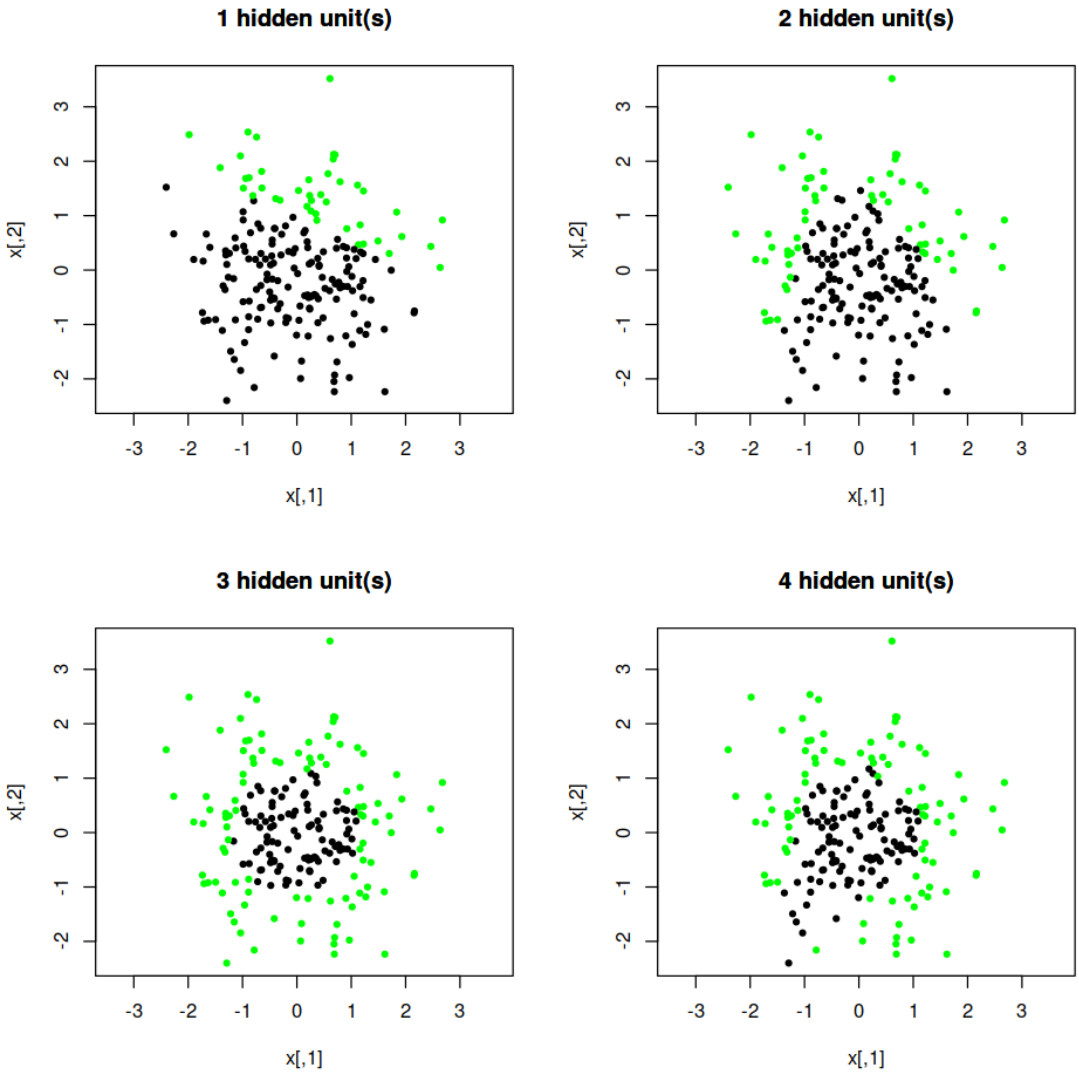
```
      predicted
actual  0  1
     0 91  9
     1  7 93
```

we see that the optimizer does not always find a good solution, even with the right number of neurons

How many hidden units do we need?

```
In [46]: options(repr.plot.width=8, repr.plot.height=8)
         par(mfrow=c(2,2))
         for (i in 1:4)
         {
           set.seed(3)
           nn1 <- nnet(y~x.1+x.2,
                       data=mydata,
                       entropy=T,
                       size=i,
                       decay=0,
                       maxit=2000,
                       trace=F)
           yhat <- as.numeric(predict(nn1,type='class'))
           plot(x,
```

```
        pch=20,
        col=c('black','green')[yhat+1],
        main=paste(i,'hidden unit(s)'),
        asp=1)
  title(main=paste(i,'hidden unit(s)'))
  }
```



Let's find out which function has been learned exactly, with 3 units

```
In [47]: set.seed(3)
         nn1 <- nnet(y~x.1+x.2,
                     data=mydata,
                     entropy=T,
                     size=3,
```

```
                    decay=0,
                    maxit=2000,
                    trace=F)
```

create a grid of values

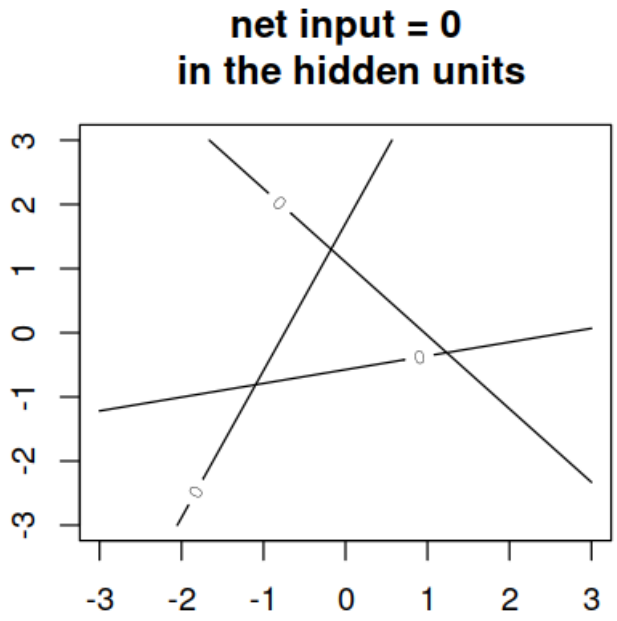
```
In [48]: x1grid <- seq(-3,3,l=200)
         x2grid <- seq(-3,3,l=220)
         xg <- expand.grid(x1grid,x2grid)
         xg <- as.matrix(cbind(1,xg))
```

input them to the hidden units, and get their outputs

```
In [49]: h1 <- xg%*%matrix(coef(nn1)[1:3],ncol=1)
         h2 <- xg%*%matrix(coef(nn1)[4:6],ncol=1)
         h3 <- xg%*%matrix(coef(nn1)[7:9],ncol=1)
```

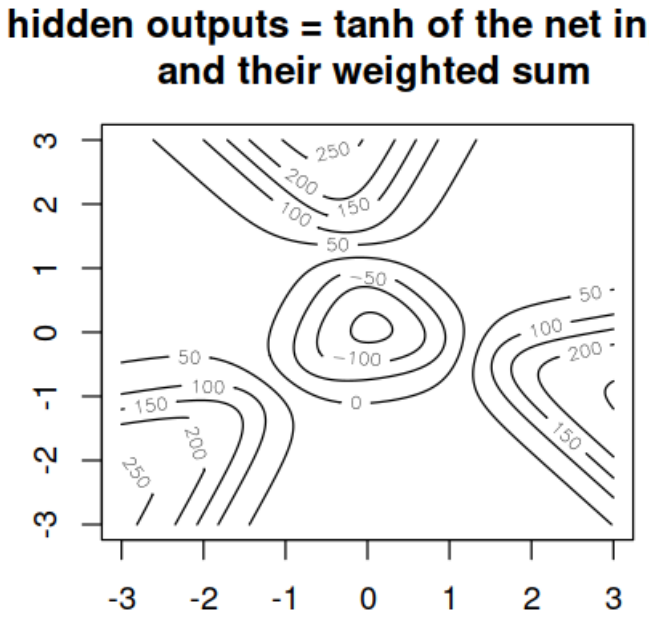
the hidden units compute the logistic() function, so we cut the output value at 0; we get a decision line

```
In [50]: options(repr.plot.width=4, repr.plot.height=4)
         par(mfrow=c(1,1))
         contour(x1grid,x2grid,matrix(h1,200,220),levels=0)
         contour(x1grid,x2grid,matrix(h2,200,220),levels=0,add=T)
         contour(x1grid,x2grid,matrix(h3,200,220),levels=0,add=T)
         title(main='net input = 0\n in the hidden units')
```

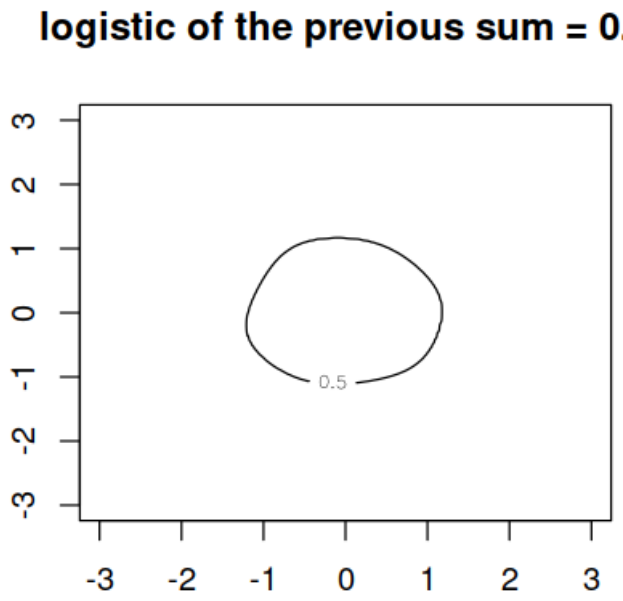


this is the logistic function, used by nnet() for the hidden neurons, and for the output neurons in two-class classification problems

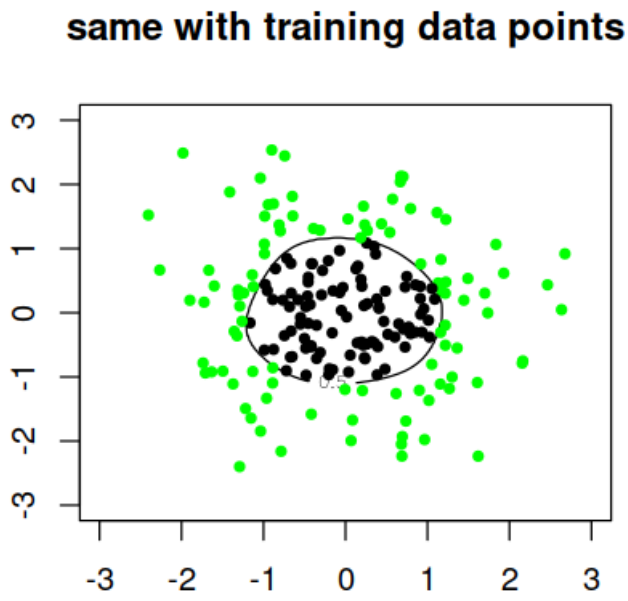
```
In [51]: logistic <- function(x) {1/(1+exp(-x))}

         z <- coef(nn1)[10] + coef(nn1)[11]*logistic(h1) +
                coef(nn1)[12]*logistic(h2) + coef(nn1)[13]*logistic(h3)

         contour(x1grid,x2grid,matrix(z,200,220))
         title('hidden outputs = tanh of the net inputs\n and their weighted sum')
```




```
In [52]: contour(x1grid,x2grid,matrix(logistic(z),200,220),levels=0.5)
         title('logistic of the previous sum = 0.5')
```



In [53]:
```
contour(x1grid,x2grid,matrix(logistic(z),200,220),levels=0.5)
points(x,pch=20,col=c('black','green')[y+1])
title('same with training data points')
```



If you prefer a more visual demo of how ANN work, you can play with the Google's tensorflow playground http://playground.tensorflow.org

---

1.3 Radial Basis Function Network Example: regression of a 1D function

```
In [54]: set.seed (4)

         library (cclust)
```

We are going to do all the computations "by hand"
Let us depart from the following function in the (a,b) interval

```
In [55]: myf <- function (x) { (1 + x - 2*x^2) * exp(-x^2) }
```

We are going to model this function in the interval (-5,5)

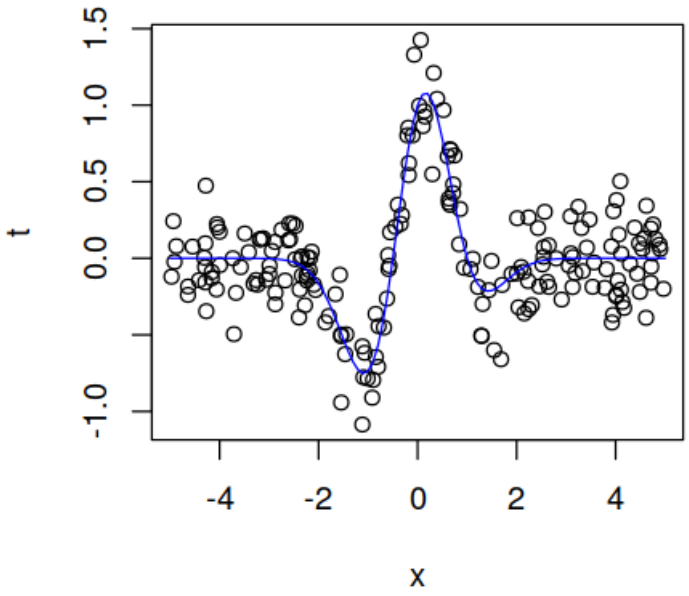
```
In [56]: a <- -5
         b <- 5

         domain <- c(a,b)

         myf.data <- function (N, a, b)
```

```
{
  x <- runif(N, a, b)
  t <- myf(x) + rnorm(N, sd=0.2)
  dd <- data.frame(x,t)
  names(dd) <- c("x", "t")
  return (dd)
}

N <- 200
d <- myf.data (N, a , b)

summary(d)
```

```
       x                   t          
 Min.   :-4.97077   Min.   :-1.08566  
 1st Qu.:-2.36338   1st Qu.:-0.20412  
 Median : 0.04794   Median :-0.04610  
 Mean   : 0.14686   Mean   : 0.00188  
 3rd Qu.: 2.64938   3rd Qu.: 0.19471  
 Max.   : 4.96613   Max.   : 1.42546  
```

The black points are the data, the blue line is the true underlying function

In [57]:
```
options(repr.plot.width=4, repr.plot.height=4)
plot (d)
curve (myf, a, b, col='blue', add=TRUE)
```



Create a large test data too for future use; notice that the generation mechanism is the same

```
In [58]: N.test <- 2000
         d.test <- myf.data (N.test, a , b)
```

Function to compute a PHI (N x M) design matrix, without the Phi_0(x) = 1 column; m.i, h.i are the centers and variances (sigmas) of the neurons, respectively

```
In [59]: PHI <- function (x,m.i,h.i)
         {
           N <- length(x)
           M <- length(m.i)
           phis <- matrix(rep(0,(M)*N), nrow=M, ncol=N)
           for (i in 1:M)
           {
             phis[i,] <- exp(-(x - m.i[i])^2/(2*h.i[i]))
           }
           t(phis)
         }
```

We find the centers and variances for each neuron using k-means; since this clustering algorithm is non-deterministic (because the initial centers are random), we do it 'NumKmeans' times

```
In [60]: NumKmeans <- 10
```

We set a rather large number of hidden units (= basis functions) M as a function of data size (the sqrt is just a heuristic!) because we are going to try different regularizers

```
In [61]: (M <- floor(sqrt(N)))

         m <- matrix(0,nrow=NumKmeans,ncol=M)
         h <- matrix(0,nrow=NumKmeans,ncol=M)

         data.Kmeans <- cbind(d$x,rep(0,N))

         for (j in 1:NumKmeans)
         {
           # Find the centers m.i with k-means
           km.res <- cclust (x=data.Kmeans,
                             centers=M,
                             iter.max=200,
                             method="kmeans",
                             dist="euclidean")
           m[j,] <- km.res$centers[,1]

           # Obtain the variances h.i as a function of the m.i
           h[j,] <- rep(0,M)
```

```
  for (i in 1:M)
  {
    indexes <- which(km.res$cluster == i)
    h[j,i] <- sum(abs(d$x[indexes] - m[j,i]))/length(indexes)
    if (h[j,i] == 0) h[j,i] <- 1
  }
}
```

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Now for each k-means we get the hidden-to-output weights by solving a regularized least-squares problem (standard ridge regression), very much as we did in previous labs

The difference is that now we perform ridge regression on the PHI matrix (that is, on the new regressors given by the hidden neurons), not on the original inputs ...

... and find the best lambda with using GCV across all choices of basis functions (the NumK-means clusterings)

In [62]:
```
(lambdes <- 10^seq(-3,1.5,by=0.1))

library(MASS) # we need it for lm.ridge

errors <- rep(0,NumKmeans)
bestLambdes <- rep(0,NumKmeans)

# For each k-means result
for (num in 1:NumKmeans)
{
  m.i <- m[num,]
  h.i <- h[num,]

  myPHI <- PHI (d$x,m.i,h.i)
  aux1 <- lm.ridge(d$t ~ myPHI, d, lambda = lambdes)
  my.lambda <- as.numeric(names(which.min(aux1$GCV)))

  aux2 <- lm.ridge(d$t ~ myPHI, d, lambda = my.lambda)

  errors[num] <- sqrt(aux2$GCV)
  bestLambdes[num] <- my.lambda

}
```

1. 0.001 2. 0.00125892541179417 3. 0.00158489319246111 4. 0.00199526231496888 5. 0.00251188643150958 6. 0.00316227766016838 7. 0.00398107170553497 8. 0.00501187233627272 9. 0.00630957344480193 10. 0.00794328234724281 11. 0.01 12. 0.0125892541179417 13. 0.0158489319246111 14. 0.0199526231496888 15. 0.0251188643150958 16. 0.0316227766016838 17. 0.0398107170553497 18. 0.0501187233627272 19. 0.0630957344480193 20. 0.0794328234724282 21. 0.1 22. 0.125892541179417 23. 0.158489319246111 24. 0.199526231496888 25. 0.251188643150958 26. 0.316227766016838 27. 0.398107170553497 28. 0.501187233627272 29. 0.630957344480194 30. 0.794328234724282 31. 1 32. 1.25892541179417 33. 1.58489319246111 34. 1.99526231496888

35. 2.51188643150958 36. 3.16227766016838 37. 3.98107170553497 38. 5.01187233627272 39. 6.30957344480194 40. 7.94328234724282 41. 10 42. 12.5892541179417 43. 15.8489319246111 44. 19.9526231496888 45. 25.1188643150958 46. 31.6227766016838

Now we obtain the best model among the tested ones

```
In [63]: bestIndex <- which(errors == min(errors))
         bestLambda <- bestLambdes[bestIndex]
         m.i <- m[bestIndex,]
         h.i <- h[bestIndex,]
```

we see that this problem needs a lot of regularization! This makes sense if you take a look at how the data is generated (the previous plot): the noise level is very high relative to the signal

We also see that the best lambda fluctuates (since the data changes due to the clustering, but the order of magnitude is quite stable

```
In [64]: bestLambdes
```

1. 1.258925412 2. 6.309573445 3. 1.258925412 4. 5.011872336 5. 3.981071706 6. 5.011872336 7. 3.16227766 8. 7.943282347 9. 6.309573445 10. 5.011872336

We now create the final model:

```
In [65]: my.RBF <- lm.ridge(d$t ~ PHI (d$x,m.i,h.i), d, lambda = bestLambda)
```

these are the final hidden-to-output weights: note how small they are (here is where we regularize)

```
In [66]: (w.i <- setNames(coef(my.RBF), paste0("w_", 0:M)))
```

w_0 0.024822089200559 **w_1** -0.0663458900997104 **w_2** 0.497416574403686 **w_3** -0.346465504483054 **w_4** 0.129436666139729 **w_5** 0.0112163267267736 **w_6** -0.106166434653156 **w_7** -0.00212525860013 **w_8** -0.441257657931165 **w_9** -0.823893755521675 **w_10** -0.110522033101117 **w_11** -0.0338083093982085 **w_12** 0.0514178316503273 **w_13** -0.114800176311969 **w_14** 0.97902198439685

It remains to calculate the prediction on the test data

```
In [67]: test.PHI <- cbind(rep(1,length(d.test$x)),PHI(d.test$x,m.i,h.i))
         y <- test.PHI %*% w.i
```

And now the normalized error of this prediction

```
In [68]: (errorsTest <- sqrt(sum((d.test$t - y)^2)/((N.test-1)*var(d.test$t))))
```

0.507681762667632

Much better if we plot everything

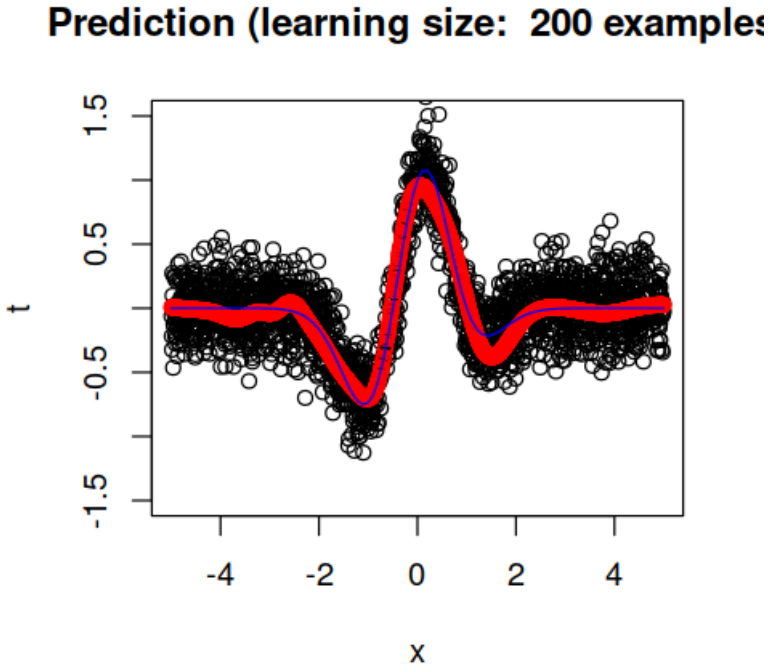
```
In [69]: par(mfrow=c(1,1))
```

Test data in black, Red data are the predictions and the blue line is the underlying function

```
In [70]: plot(d.test$x,d.test$t,
              xlab="x",ylab="t",
              main=paste("Prediction (learning size: ",toString(N),"examples)"),
              ylim=c(-1.5,1.5))

         points(d.test$x,y,col='red',lwd=1)

         curve (myf, a, b, col='blue', add=TRUE)
```



The previous code is designed for 1D problems but you can easily adapt it to more input dimensions

There is a general package for neural networks: {RSNNS}

Which is actually the R interface to the (formerly widely used and flexible) Stuttgart Neural Network Simulator (SNNS)

This library contains many standard implementations of neural networks. The {RSNNS} package actually wraps the SNNS functionality to make it available from within R

The RBF version within this package has a sophisticated method for initializing the network, which is also quite non-standard, so we avoid further explanation

Sadly this package does not provide with a way to control regularization or to allow for multi-class problems (a softmax option with the cross-entropy would be welcome)