Math 5365

Data Mining 1

Homework 14

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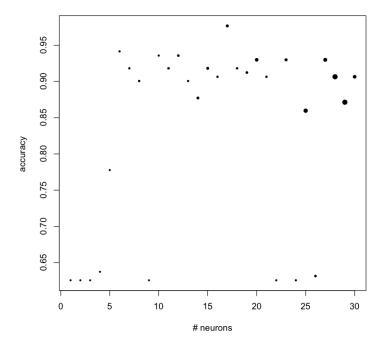
1. Use gradient descent to minimize the function $f(x,y) = x^2 + y^2 + y$ on the open disk $x^2 + y^2 < 1$. This is essentially the example on p. 7 of the Lagrange multipliers slides, except that we are only interested in interior points on this problem.

(Hints: Start by randomly selecting a vector (x, y) in the disk, and then apply gradient descent. If the vector excapes the disk during the algorithm, randomly select a new vector. Store vectors that converge to a minimum in a matrix, and repeat the entire process a large number of times to ensure that there is only one local minimum inside the disk. You may need to take some care with the learning rate to prevent vectors from escaping the disk too often.)

Using 300 initial guesses, the gradient descent function accurately computed the minimum point and gradient to within 10e-10 accuracy.

2. Compare the merits of using a 2-layer neural network (with 1 hidden layer) and a multi-layer neural network to the wdbc data set. Let's say you only have 10 minutes to train a network with nnet or mlp. Which approach produces the model with the higher classification accuracy? It may be interesting to compare the two packages for a variety of time frames and to consider different network topologies for mlp, e.g., size=c(2, 4) vs. size=c(2, 2, 2).

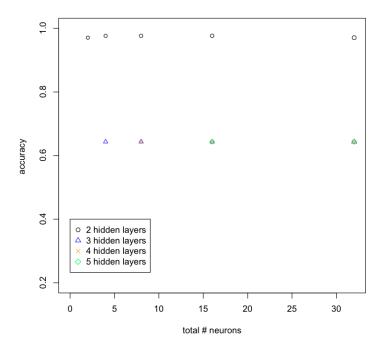
The first thing I considered was the effect of increasing the size of the hidden layer. The results, together with total time taken for each corresponding model are shown below. Note that the size of the data point corresponds to the length of time taken to produce the model.



As can be seen, the overall runtime increases with the size of the hidden layer. However, the accuracy also increases dramatically between 1 and 5 neurons and then remains largely at the same level (with variation). The highest accuracy occured when using 17 neurons. With this model, the accuracy was approximately 98%. The total time taken for this model is slightly above average at a value of 0.254 seconds where the maximum time taken was 0.799 seconds, the minimum time taken was 0.008, and the mean time was 0.1976 seconds.

For the multi-layer neural networks, I compared results using 2 through 5 hidden layers. In each case, the number of neurons in each layer was equal. Thus for a network with 4 hidden layers and 16 total neurons, each layer contains 4 neurons.

The results are shown in the graph below. As in the single hidden layer case above, the size of the point indicates the length of time taken to create the model.



The average time taken was 0.8603333 seconds, with a minimum of 0.818 seconds using a neural network with 4 hidden layers and 1 neuron in each layer, and a maximum of 1.022 seconds for a neural network with 2 hidden layers and 8 neurons in each layer. The variations in time with these cases are so small that time taken has little meaning except when compared with the case of a single hidden network.

The maximum accuracy using multi-layer neural networks was roughly 98%, the same as for 1 hidden layer. This level of accuracy was achieved using 4 neurons in each case. Thus it can be seen that for this problem, the most accurate models are not the most complex ones, but rather the single- and double-hidden layer models. In addition, the most time-efficient model is the single-layer model. Therefore the best model for this problem is a network with a single hidden layer and 4 neurons.

² library(doMC)

³ registerDoMC()

```
4
   source('~/Dropbox/Tarleton/data_mining/generic_functions/dataset_ops.R')
   #1 Use gradient descent to minimize the function f(x, y) = x^2 + y^2 + y
      on the open disk x^2 + y^2 < 1. This is essentially the example on
      p. 7 of the Lagrange multipliers slides, except that we are only
      interested in interior points on this problem.
10
11
      (Hints: Start by randomly selecting a vector (x, y) in the disk, and
       then apply gradient descent. If the vector excapes the disk during the
   #
13
       algorithm, randomly select a new vector. Store vectors that converge
   #
   #
       to a minimum in a matrix, and repeat the entire process a large number
15
   #
       of times to ensure that there is only one local minimum inside the disk.
16
   #
       You may need to take some care with the learning rate to prevent vectors
   #
       from escaping the disk too often.)
18
   f <- function(x){</pre>
20
     return( sum(x^2) + x[2])
   }
22
23
   grad_f <- function(x){</pre>
24
      return(c(2*x[1], 2*x[2] + 1))
25
   }
26
27
   params <- function(x){</pre>
     if (sum(x^2) < 1){
29
             return(TRUE)
30
```

```
}else{
31
               return(FALSE)
32
      }
33
   }
34
35
   initial_guess <- function(){</pre>
36
      x \leftarrow runif(2, -1, 1)
      return(x)
38
   }
39
40
   grad_descent <- function(f, grad_f, params, initial_guess, x0, eps, tol, niter){</pre>
41
      i = 1; NOT_ZERO = TRUE
^{42}
      x = x0
43
      while((i < niter) && (NOT_ZERO)){</pre>
44
        i = i + 1
45
        xo = x
46
        x = xo - eps * grad_f(x)
47
        if(f(x) < f(xo)){
                    eps = eps * 1.1
49
        }else{
50
                   eps = eps * 0.5
51
                 }
52
        if(params(x)){
53
          if(abs(sum(grad_f(x)^2)) < tol){
54
             NOT_ZERO = FALSE
          }
56
        }else{
```

```
x <- initial_guess()</pre>
58
        eps = 0.75 * eps
59
        i = 1
60
      }
61
    }
62
    return(list(grad = grad_f(x), x = x, dx = eps,
63
                nit = i, converged = !NOT_ZERO))
64
  }
65
66
  67
  # Initialize matrix of initial guesses and compute gradient descent
68
  69
  n_{guesses} = 300
70
  x_m <- matrix(runif(n_guesses * 2, -1, 1), nrow = n_guesses, ncol = 2)</pre>
  vals <- matrix(,nrow=n_guesses,ncol=2)</pre>
72
  vals <- foreach(i=1:n_guesses, .combine=rbind) %dopar% {</pre>
74
    grad_descent(f, grad_f, params, initial_guess, x_m[i,], 0.9, 1.0e-17, 10000)$x
  }
76
77
  dx <- paste('TOTAL VARIATION IN COMPUTED CRITICAL POINT',</pre>
78
              '\n variation in x-values -> ',
79
              toString(max(vals[,1]) - min(vals[,1])),
80
              '\n','variation in y-values -> ',
81
               toString(max(vals[,2]) - min(vals[,2])))
82
  writeLines(dx)
83
  print(apply(vals, 1, grad_f))
```

```
85
    #2 Compare the merits of using a 2-layer neural network (with 1 hidden layer)
86
       and a multi-layer neural network to the wdbc data set. Let's say you only
    #
       have 10 minutes to train a network with nnet or mlp. Which approach produces
88
       the model with the higher classification accuracy? It may be interesting to
89
       compare the two packages for a variety of time frames and to consider
90
       different network topologies for mlp, e.g., size=c(2, 4) vs. size=c(2, 2, 2).
91
92
    library(nnet)
93
    library(RSNNS)
94
95
    source('~/Dropbox/Tarleton/data_mining/class_notes/extras.R')
96
    wdbc <- read.csv('~/Dropbox/Tarleton/data_mining/dfiles/wdbc.data',</pre>
97
                       header=F, sep=',')
98
    wdbc <- wdbc[,-1]
99
    splitset <- splitdata(wdbc,0.7,F)</pre>
100
    train <- splitset$train</pre>
101
102
    ## Consider first merely increasing size
103
    len = 30
104
105
106
    # 1
          2
                        8
                                   16
107
                 22
    #
         11
                        44
                                  88
108
                       2222
                                 4444
    #
                1111
109
                     11111111 2222222
    #
110
   #
                           11111111111111111
111
```

```
112
    # accnnet <- rep(-1,len)</pre>
113
    # for(i in 1:len){
114
      # model <- nnet(V2~., wdbc[train,], size=i,trace=F)</pre>
115
      # predvals <- predict(model,wdbc[-train,],type='class')</pre>
116
      # accnnet[i] <- confmatrix(wdbc$V2[-train], predvals)$accuracy</pre>
117
    # }
118
119
    normwdbc <- standardize(wdbc, 2:ncol(wdbc))</pre>
120
    train_vals <- normwdbc[train,-1]</pre>
121
    train_targ <- decodeClassLabels(normwdbc[train,1])</pre>
122
    test_vals <- normwdbc[-train,-1]</pre>
123
    test_targ <- decodeClassLabels(normwdbc[-train,1])</pre>
124
125
    num = 4
126
    accnnet <- rep(-1, num)</pre>
127
    accmlpnet <- matrix(-1, num, num)</pre>
128
    nnet_times <- rep(-1, num)</pre>
129
    mlp_times <- matrix(-1, num, num)</pre>
130
131
    for(i in 1:num){
132
      t_0 <- proc.time()
133
      model <- nnet(V2~., wdbc[train,], size=i, linout=F, trace=F)</pre>
134
      t_1 <- proc.time()
135
      nnet_times[i] \leftarrow t_1[3] - t_0[3]
136
      predvals <- predict(model, wdbc[-train,],type='class')</pre>
137
      accnnet[i] <- confmatrix(wdbc$V2[-train], predvals)$accuracy</pre>
138
```

```
139
      for(j in 1:num){
140
         if(j \ge i){
141
           reps <- 2^(i - 1)
142
           vec \leftarrow rep(2^(j - i), reps)
143
           t_0 <- proc.time()</pre>
144
           model <- mlp(train_vals,</pre>
145
                           train_targ,
146
                           size=vec,
147
                           maxit = 50,
148
                           learnFuncParams = c(0.1),
149
                           inputsTest = test_vals,
150
                           targetsTest = test_targ,
151
                           linout = TRUE)
152
           t_1 <- proc.time()
153
           mlp_times[i,j] \leftarrow t_1[3] - t_0[3]
154
           idx <- (model$fittedTestValues[,1] >= 0.5) * 1
155
           predvals <- idx</pre>
156
           predvals[idx == 1] <- 'B'</pre>
157
           predvals[idx == 0] <- 'M'</pre>
158
           accmlpnet[i,j] <- confmatrix(wdbc$V2[-train], predvals)$accuracy</pre>
159
         }
160
      }
161
    }
162
    mlp_times
163
```