Neural Networks (2014)
Practical Assignment III: Learning by gradient descent

Stochastic gradient descent
The aim of this problem is to get acquainted with gradient descent based training in practice and do some *hands on* experiments. Take the actual assignment as a starting point for further exploration and self-study.
We consider a simple feedforward neural network with real-valued output

$$\sigma(\boldsymbol{\xi}) = (\tanh[\boldsymbol{w}_1 \cdot \boldsymbol{\xi}] + \tanh[\boldsymbol{w}_2 \cdot \boldsymbol{\xi}])$$

where $\boldsymbol{\xi} \in I\!R^N$ represents an input vector and $\boldsymbol{w}_1$ and $\boldsymbol{w}_2$ are the N-dim. vectors of adaptive input–to–hidden weights. The fixed hidden-to-output relation is given as the sum of the hidden states *(soft committee machine)*.

a) Stochastic gradient descent
Formulate and implement a stochastic gradient descent procedure w.r.t. the weight vectors $\boldsymbol{w}_1$ and $\boldsymbol{w}_2$, which aims at the minimization of the cost function

$$E = \frac{1}{P}\frac{1}{2}\sum_{\mu=1}^{P}\left(\sigma(\boldsymbol{\xi}^\mu) - \tau(\boldsymbol{\xi}^\mu)\right)^2$$

for a given data set $I\!D = \{\boldsymbol{\xi}^\mu, \tau(\boldsymbol{\xi}^\mu)\}_{\mu=1}^{P}$ with continuous training labels $\tau(\boldsymbol{\xi}^\mu) \in I\!R$.
In each learning step, select one of the P examples, say $\boldsymbol{\xi}^\nu$, randomly with equal probability and use the gradient with respect to its contribution $e^\nu = (\sigma(\boldsymbol{\xi}^\nu) - \tau(\boldsymbol{\xi}^\nu))^2/2$, only (stochastic gradient descent):

$$\begin{aligned}\boldsymbol{w}_1 &\leftarrow \boldsymbol{w}_1 - \eta\, \nabla_{\boldsymbol{w}_1} e^\nu \\ \boldsymbol{w}_2 &\leftarrow \boldsymbol{w}_2 - \eta\, \nabla_{\boldsymbol{w}_2} e^\nu\end{aligned}$$

where $\nabla_{\boldsymbol{w}_j}$ denotes the gradient with respect to $\boldsymbol{w}_j$.
Perform $t_{max} \cdot P$ single training steps, where $t \leq t_{max}$ measures the *training time* in units of P single updates.
Initialize the weights as independent random vectors with $|\boldsymbol{w}_1|^2 = 1$ and $|\boldsymbol{w}_2|^2 = 1$. You can work with a constant learning rate. A reasonable choice of the learning rate should be $\eta = 0.05$, but you may want to use different values, depending on the observed performance.

b) A regression problem
In Nestor you will find the file `data3.mat` which you should import into Matlab (`load data3.mat`). It provides a 50×5000-dim. array `xi` corresponding to 5000 input vectors (dimension $N = 50$) and a 5000-dim. vector `tau` corresponding to the target values.
Consider (at least) the first $P = 100$ examples as the training set.
In the course of stochastic gradient descent training, measure the cost function E and plot it vs. the time t as defined above.
In addition, evaluate the quantity

$$E_{test} = \frac{1}{Q}\frac{1}{2}\sum_{\rho=P+1}^{P+Q}\left(\sigma(\boldsymbol{\xi}^\rho) - \tau(\boldsymbol{\xi}^\rho)\right)^2$$

which corresponds to the *test* or *generalization error* in terms of quadratic deviation from the target function for Q test examples, set $Q = 100$ or larger.
Plot and compare the evolution of E and E_{test} with the training time t. You should consider training times t_{max} after which the errors seem to have become roughly constant (apart from

fluctuations). Display the obtained, final weight vectors as bar graphs.

Hand in at least the following:

- A brief description of the problem, including the update equations according to stochastic gradient descent
- The curves $E(t)$ and $E_{test}(t)$ corresponding to the above specified (or similar) parameters
- Bar graphs displaying the two weight vectors after t_{max}

Remarks:

- You can follow the supplementary material (grad-example.pdf) in Nestor for the calculation of derivatives. Note, however, that here hidden-to-output weights and the gain parameters are fixed.
- If you want to solve the problem using some other programming language you can export the arrays in text or csv format from within matlab using the commands `save` or `csvwrite`, for instance. See the matlab documentation for syntax and options.
- You could also consider the concatenated vector $\underline{W} = [\boldsymbol{w}_1, \boldsymbol{w}_2]$ and use the gradient with respect to $\underline{W}$, but since $\nabla_{\underline{W}} = [\nabla \boldsymbol{w}_1, \nabla \boldsymbol{w}_2]$ this is completely equivalent to the above.
- Compute E and E_{test} after P single randomized steps, not after each individual update.
- Of course, your results will be more reliable if you repeat the training process over several runs from random initializations and take an average of $E(t)$ and $E_{test}(t)$ over these runs. However, this is not obligatory and depends on your patience and and available CPU time.

Possible bonus problems

- consider smaller and larger values of P, e.g. a selection from $P = 20, 50, 200, 500, 1000, 2000$ for the training process. How do the final training and test errors depend on P? Make sure that the Q test examples are not used in the training, of course.
- study systematically the influence of the learning rate η. Potentially consider a time dependent rate as discussed in class.
- Can you observe plateau states? If so, display the corresponding weight vectors and compare with the final ones after leaving the plateau.
- consider a student network with $K > 2$ for the same data set. Can you observe over-fitting?
- ...