MATH 567: Mathematical Techniques in Data Science
Lab 8

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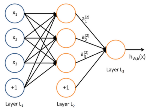
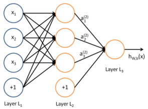
Recall



We have:

$$\begin{aligned}
a_1^{(2)} &= f(W_{11}^{(1)} x_1 + W_{12}^{(1)} x_2 + W_{13}^{(1)} x_3 + b_1^{(1)}) \\
a_2^{(2)} &= f(W_{21}^{(1)} x_1 + W_{22}^{(1)} x_2 + W_{23}^{(1)} x_3 + b_2^{(1)}) \\
a_3^{(2)} &= f(W_{31}^{(1)} x_1 + W_{32}^{(1)} x_2 + W_{33}^{(1)} x_3 + b_3^{(1)}) \\
h_{W,b} = a_1^{(3)} &= f(W_{11}^{(2)} a_1^{(2)} + W_{12}^{(2)} a_2^{(2)} + W_{13}^{(2)} a_3^{(2)} + b_1^{(2)}).
\end{aligned}$$

Recall (cont.)



Vector form:

$$\begin{aligned}
z^{(2)} &= W^{(1)} x + b^{(1)} \\
a^{(2)} &= f(z^{(2)}) \\
z^{(3)} &= W^{(2)} a^{(2)} + b^{(2)} \\
h_{W,b} = a^{(3)} &= f(z^{(3)}).
\end{aligned}$$

Training neural networks

Suppose we have

- A neural network with s_l neurons in layer l ($l = 1, \dots, n_l$).
- Observations $(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)}) \in \mathbb{R}^{s_1} \times \mathbb{R}^{s_{n_l}}$.

We would like to choose $W^{(l)}$ and $b^{(l)}$ in some optimal way for all l.

Let

$$J(W, b; x, y) := \frac{1}{2} \|h_{W,b}(x) - y\|_2^2 \qquad \text{(Squared error for one sample).}$$

Define

$$J(W, b) := \frac{1}{m} \sum_{i=1}^{m} J(W, b; x^{(i)}, y^{(i)}) + \frac{\lambda}{2} \sum_{l=1}^{n_l - 1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} (W_{ji}^{(l)})^2.$$

(average squared error with Ridge penalty).

Note:

- The Ridge penalty prevents overfitting.
- We do not penalize the bias terms $b_i^{(l)}$.

Some remarks

- Can use other loss functions (e.g. for classification).
- Can use other penalties (e.g. ℓ_1, elastic net, etc.).
- In classification problems, we choose the labels $y \in \{0, 1\}$ (if working with sigmoid) or $y \in \{-1, 1\}$ (if working with $\tanh$).
- For regression problems, we scale the output so that $y \in [0, 1]$ (if working with sigmoid) or $y \in [-1, 1]$ (if working with $\tanh$).
- We can use gradient descent to minimize $J(W, b)$. Note that since the function $J(W, b)$ is non-convex, we may only find a *local* minimum.
- We need an initial choice for $W_{ij}^{(l)}$ and $b_i^{(l)}$. If we initialize all the parameters to 0, then the parameters remain constant over the layers because of the symmetry of the problem.
- As a result, we initialize the parameters to a small constant at random (say, using $N(0, \epsilon^2)$ for $\epsilon = 0.01$).

Gradient descent and the backpropagation algorithm

- We update the parameters using a gradient descent as follows:

$$W_{ij}^{(l)} \leftarrow W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$
$$b_i^{(l)} \leftarrow b_i^{(l)} - \alpha \frac{\partial}{\partial b_i^{(l)}} J(W, b).$$

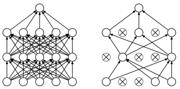
Here $\alpha > 0$ is a parameter (the *learning rate*).

- The partial derivatives can be cleverly computed using the chain rule to avoid repeating calculations (backpropagation algorithm).

Sparse neural networks

Sparse networks can be built by

- Penalizing coefficients (e.g. using a ℓ_1 penalty).
- Dropping some of the connections at random (dropout).



Srivastava et al., JMLR 15 (2014).

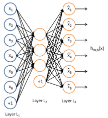
Useful to prevent overfitting.

Recent work: "One-shot learners" can be used to train models with a smaller sample size.

Autoencoders

An **autoencoder** learns the identity function:

- Input: unlabeled data.
- Output = input.
- Idea: limit the number of hidden layers to discover structure in the data.
- Learn a *compressed* representation of the input.



Source: UFLDL tutorial.

Example (UFLDL)

- Train an autoencoder on 10×10 images with one hidden layer.
- Each hidden unit i computes:

$$a_i^{(2)} = f\left(\sum_{j=1}^{100} W_{ij}^{(1)} x_j + b_j^{(1)}\right).$$

- Think of $a_i^{(2)}$ as some non-linear feature of the input x.

Problem: Find x that maximally activates $a_i^{(2)}$ over $\|x\|_2 \leq 1$.

Claim:

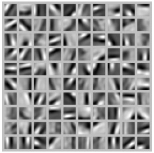
$$x_j = \frac{W_{ij}^{(1)}}{\sqrt{\sum_{j=1}^{100} (W_{ij}^{(1)})^2}}.$$

(Hint: Use Cauchy–Schwarz).

We can now display the image maximizing $a_i^{(2)}$ for each i.

Example (cont.)

100 hidden units on 10x10 pixel inputs:



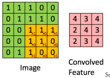
The different hidden units have learned to detect edges at different positions and orientations in the image.

Using convolutions

- Idea: Certain signals are *stationary*, i.e., their statistical properties do not change in space or time.
- For example, images often have similar statistical properties in different regions in space.
- That suggests that the features that we learn at one part of an image can also be applied to other parts of the image.
- Can "convolve" the learned features with the larger image.

Example: 96×96 image.

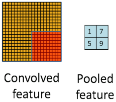
- Learn features on small 8×8 patches sampled randomly (e.g. using a sparse autoencoder).
- Run the trained model through all 8×8 patches of the image to get the feature activations.



Source: UFLDL tutorial.

Pooling features

- Once can also *pool* the features obtained via convolution.
- For example, to describe a large image, one natural approach is to aggregate statistics of these features at various locations.
- E.g. compute the mean, max, etc. over different regions.
- Can lead to more robust features. Can lead to invariant features.
- For example, if the pooling regions are contiguous, then the pooling units will be "translation invariant", i.e., they won't change much if objects in the image are undergo a (small) translation.



R

We will use the package `h2o` to train neural networks with `R`. To get you started, we will construct a neural network with 1 hidden layers containing 2 neurons to learn the XOR function:

	0	1
0	0	1
1	1	0

```
# Initialize h2o
library(h2o)

h2o.init(nthreads=-1, max_mem_size="2G")
h2o.removeAll() # in case the cluster was
                # already running

# Construct the XOR function
X = t(matrix(c(0,0,0,1,1,0,1,1),2,4))
y = matrix(c(-1,1,1,-1), 4)
train = as.h2o(cbind(X,y))
```


R (cont.)

Training the model:

```
# Train model
model <- h2o.deeplearning(x = names(train)[1:2],
                          y = names(train)[3],
                          training_frame = train,
                          activation = "Tanh",
                          hidden = c(2),
                          input_dropout_ratio = 0.0,
                          l1 = 0,
                          epochs = 10000)

# Test the model
h2o.predict(model, train)
```

Some options you may want to use when building more complicated models for data:

```
activation = "RectifierWithDropout"
input_dropout_ratio = 0.2
l1 = 1e-5
```