Single Layer Networks (2)
Stochastic gradient descent; Classification

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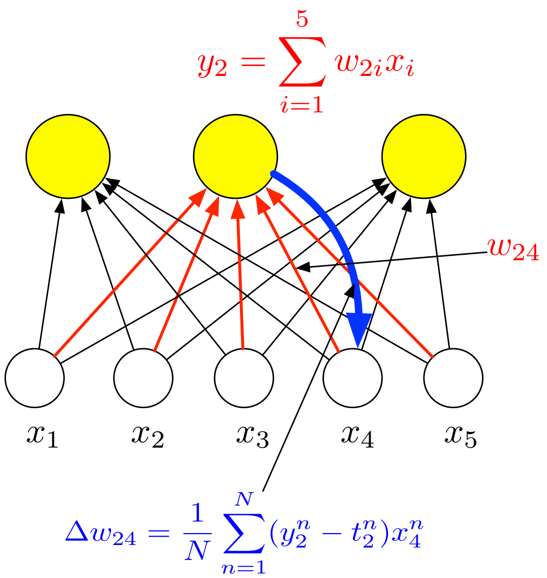
Machine Learning Practical — MLP Lecture 2
27 September 2017

Single Layer Networks

Recap: Gradient descent for a single-layer network



Stochastic Gradient Descent (SGD)

- Training by batch gradient descent is *very slow* for large training data sets
  - The algorithm sums the gradients over the entire training set before making an update
  - Since the update steps (η) are small many updates are needed
- Solution: **Stochastic Gradient Descent (SGD)**
- In SGD the true gradient $\partial E / \partial w_{ki}$ (obtained by averaging over the entire training dataset) is approximated by the gradient for a point $\partial E^n / \partial w_{ki}$
- The weights are updated after each training example rather than after the batch of training examples
- Inaccuracies in the gradient estimates are washed away by the many approximations
- To prevent multiple similar data points (all with similar gradient approximation inaccuracies) appearing in succession, present the training set in random order

SGD Pseudocode (linear network)

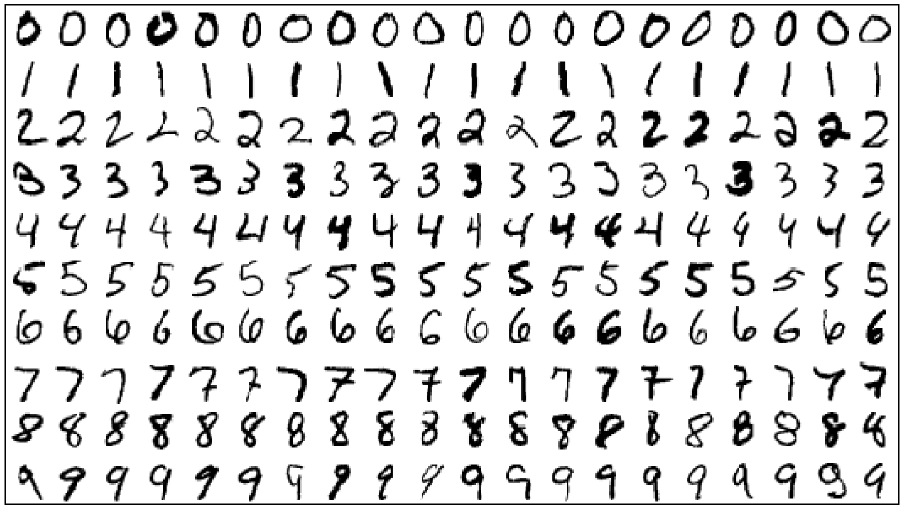
procedure $\textsc{SGDTraining}(\mathbf{X}, \mathbf{T}, \mathbf{W})$
    initialize $\mathbf{W}$ to small random numbers
    randomize order of training examples in $\mathbf{X}$
    while not converged **do**
        for $n \leftarrow 1, N$ **do**
            for $k \leftarrow 1, K$ **do**
                $y_k^n \leftarrow \sum_{i=1}^{d} w_{ki} x_i^n + b_k$
                $g_k^n \leftarrow y_k^n - t_k^n$
                for $i \leftarrow 1, d$ **do**
                    $w_{ki} \leftarrow w_{ki} - \eta \cdot g_k^n \cdot x_i^n$
                end for
                $b_k \leftarrow b_k - \eta \cdot g_k^n$
            end for
        end for
    end while
end procedure

Minibatches

- Batch gradient descent – compute the gradient from the batch of N training examples
- Stochastic gradient descent – compute the gradient from 1 training example each time
- Intermediate – compute the gradient from a **minibatch** of M training examples – $M > 1$, $M << N$
- Benefits of minibatch:
  - Computationally efficient by making best use of vectorisation, keeping processor pipelines full
  - Possibly smoother convergence as the gradient estimates are less noisy than using a single example each time

Classification

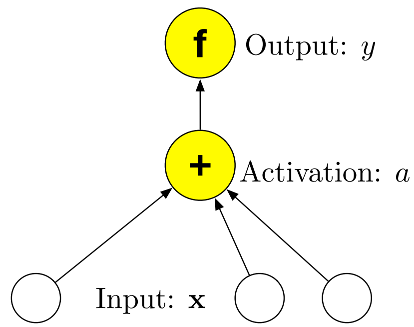
MNIST Digit Classification



Classification and Regression

- **Regression**: predict the value of the output given an example input vector - e.g. what will be tomorrow's rainfall (in mm)
- **Classification**: predict the category given an example input vector – e.g. will it be rainy tomorrow (yes or no)?
- Classification outputs:
  - **Binary**: 1 (yes) or 0 (no)
  - **Probabilistic**: p, $1-p$ (for a 2-class problem)
- One could train a linear single layer network as a classifier:
  - Output targets are 1/0 (yes/no)
  - At run time if the output $y > 0.5$ classify as yes, otherwide classify as no
- This will work, but we can do better....
- Output activation functions to constrain the outputs to binary or probabilistic (logistic / sigmoid)

Two-class classification

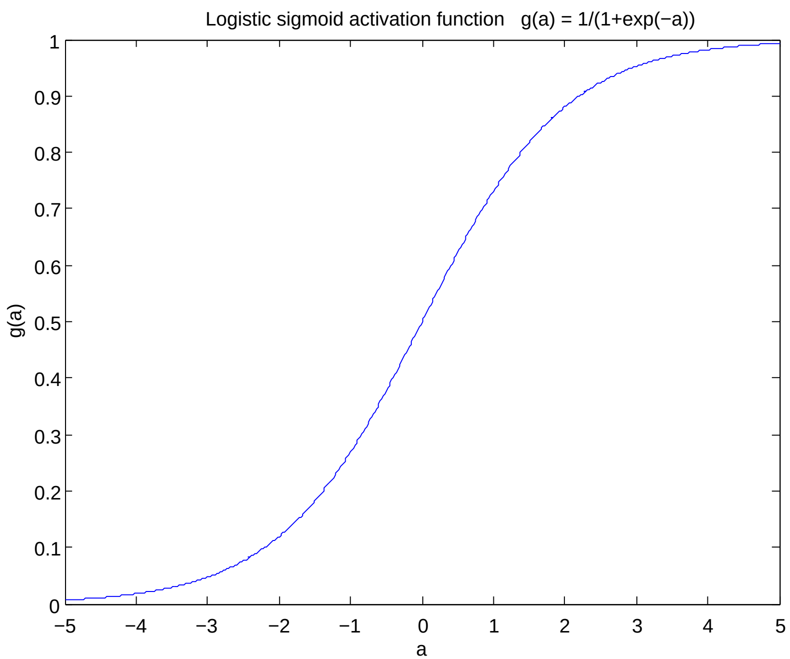


Single-layer network, binary/sigmoid output

Binary (step function): $f(a) = \begin{cases} 1 & \text{if } a \geq 0.5 \\ 0 & \text{if } a < 0.5 \end{cases}$

Probabilistic (sigmoid function): $\boxed{f(a) = \dfrac{1}{1+\exp(-a)}}$

Sigmoid function



Sigmoid single layer networks

- Binary output: activation is not differentiable. Can use *perceptron learning* to train binary output single layer networks
- Probabilistic output: sigmoid single layer network (statisticians would call this logistic regression). Let a be the *activation* of the single output unit, the value of the weighted sum of inputs, before the activation function, so:

$$y = f(a) = f\left(\sum_i w_i x_i + b\right)$$

- Two classes, so single output y, with weights w_i

Sigmoid single layer networks

- Training sigmoid single layer network: Gradient descent requires $\partial E / \partial w_i$ for all weights:

$$\frac{\partial E^n}{\partial w_i} = \frac{\partial E^n}{\partial y^n} \frac{\partial y^n}{\partial a^n} \frac{\partial a^n}{\partial w_i}$$

For a sigmoid:

$$y = f(a) \quad \frac{dy}{da} = f(a)(1 - f(a))$$

(Show that this is indeed the derivative of a sigmoid.)

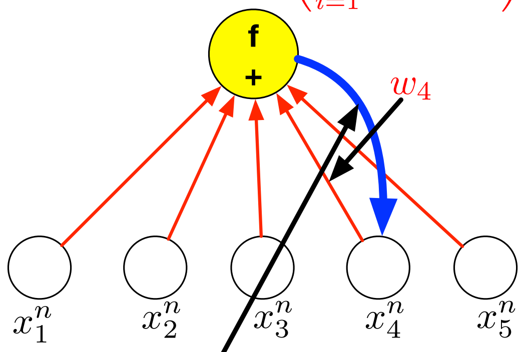
- Therefore gradients of the error w.r.t. weights and bias:

$$\boxed{\frac{\partial E^n}{\partial w_i}} = (y^n - t^n)\underbrace{f(a^n)(1 - f(a^n))}_{f'(a^n)} x_i^n$$

$$\boxed{\frac{\partial E^n}{\partial b}} = (y^n - t^n) f(a^n)(1 - f(a^n))$$

Applying gradient descent to a sigmoid single-layer network

$$y^n = f\left(\sum_{i=1}^{5} w_i x_i^n + b\right)$$



$$w_4 = w_4 - \eta(y^n - t^n)\underbrace{y^n(1 - y^n)}_{f'(a^n)} x_4^n$$

Cross-entropy error function (1)

- If we use a sigmoid single layer network for a two class problem (C_1 (target $t = 1$) and C_2 ($t = 0$)), then we can interpret the output as follows

$$y \sim P(C_1 \mid \mathbf{x}) = P(t = 1 \mid \mathbf{x})$$
$$(1 - y) \sim P(C_2 \mid \mathbf{x}) = P(t = 0 \mid \mathbf{x})$$

- Combining, and recalling the target is binary

$$P(t \mid x, \mathbf{W}) = y^t \cdot (1 - y)^{1-t}$$

This is a Bernoulli distribution. We can write the log probability:

$$\ln P(t \mid x, \mathbf{W}) = t \ln y + (1 - t) \ln(1 - y)$$

Cross-entropy error function (2)

- Optimise the weights $\mathbf{W}$ to maximise the log probability – or to minimise the negative log probability.

$$E^n = -(t^n \ln y^n + (1 - t^n) \ln(1 - y^n)) \ .$$

This is called the **cross-entropy error function**

- Gradient descent training requires the derivative $\partial E / \partial w_i$ (where w_i connects the ith input to the single output).

$$\frac{\partial E}{\partial y} = -\frac{t}{y} + \frac{1 - t}{1 - y} = \frac{-(1 - y)t + y(1 - t)}{y(1 - y)} = \frac{(y - t)}{y(1 - y)}$$

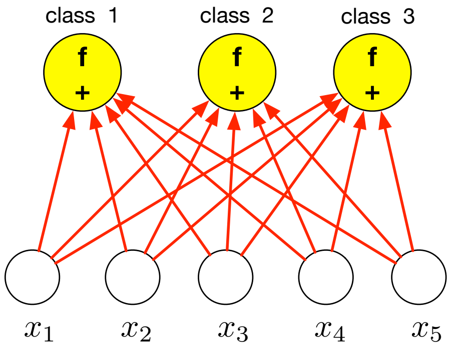
$$\boxed{\frac{\partial E}{\partial w_i}} = \frac{\partial E}{\partial y} \cdot \frac{\partial y}{\partial a} \cdot \frac{\partial a}{\partial w_i}$$

$$= \frac{(y - t)}{y(1 - y)} \cdot y(1 - y) \cdot x_i = \boxed{(y - t) x_i}$$

Derivative of the sigmoid $y(1 - y)$ cancels.
Exercise: What is the gradient for the bias ($\frac{\partial E}{\partial b}$)?

Multi-class networks

- If we have K classes use a "one-from-K" ("one-hot") output coding – target of the correct class is 1, all other targets are zero
- It is possible to have a multi-class net with sigmoids



Multi-class networks

- If we have K classes use a "one-hot" ("one-from-N") output coding – target of the correct class is 1, all other targets are zero
- It is possible to have a multi-class net with sigmoids
- This will work... but we can do better
- Using multiple sigmoids for multiple classes means that $\sum_k P(k|\mathbf{x})$ is not constrained to equal 1 – we want this if we would like to interpret the outputs of the net as class probabilities
- Solution – an activation function with a sum-to-one constraint: **softmax**

Softmax

$$\boxed{y_k = \frac{\exp(a_k)}{\sum_{j=1}^{K} \exp(a_j)}}$$

$$a_k = \sum_{i=1}^{d} w_{ki} x_i + b_k$$

- This form of activation has the following properties
  - Each output will be between 0 and 1
  - The denominator ensures that the K outputs will sum to 1
- Using softmax we can interpret the network output y_k^n as an estimate of $P(k|\mathbf{x}^n)$
- Softmax is the multiclass version of the two-class sigmoid

Softmax – Training (1)

- We can extend the cross-entropy error function to the multiclass case

$$E^n = -\sum_{k=1}^{C} t_k^n \ln y_k^n$$

- Again the overall gradients we need are

$$\boxed{\frac{\partial E^n}{\partial w_{ki}}} = \sum_{c=1}^{C} \frac{\partial E}{\partial y_c} \cdot \frac{\partial y_c}{\partial a_k} \cdot \frac{\partial a_k}{\partial w_{ki}} = \sum_{c=1}^{C} -\frac{t_c}{y_c} \cdot \frac{\partial y_c}{\partial a_k} \cdot x_i$$

$$\boxed{\frac{\partial E^n}{\partial b_k}} = \sum_{c=1}^{C} \frac{\partial E}{\partial y_c} \cdot \frac{\partial y_c}{\partial a_k} \cdot \frac{\partial a_k}{\partial b_k} = \sum_{c=1}^{C} -\frac{t_c}{y_c} \cdot \frac{\partial y_c}{\partial a_k}$$

Softmax – Training (2)

- Note that the kth activation a_k – and hence the weight w_{ki} – influences the error function through all the output units, because of the normalising term in the denominator. We have to take this into account when differentiating.
- If you do the differentiation you will find:

$$\frac{\partial y_c}{\partial a_k} = y_c(\delta_{ck} - y_k)$$

  Where δ_{ck} ($\delta_{ck} = 1$ if $c = k$, $\delta_{ck} = 0$ if $c \neq k$) is called the Kronecker delta
- We can put it all together to find:

$$\boxed{\frac{\partial E^n}{\partial w_{ki}}} = (y_k^n - t_k^n)x_i^n \qquad \boxed{\frac{\partial E^n}{\partial b_k}} = (y_k^n - t_k^n)$$

  Softmax output with cross-entropy error function results in gradients the same as for linear outputs with sum-square error!

Exercises

1. Modify the SGD pseudocode for sigmoid outputs
2. Modify the SGD pseudocode for softmax outputs
3. For softmax and cross-entropy error, show that

$$\frac{\partial E^n}{\partial w_{ki}} = (y_k^n - t_k^n)x_i^n$$

   (use the quotient rule of differentiation, and the fact that $\sum_{c=1}^{K} t_c y_k = y_k$ because of 1-from-K coding of the target outputs)

Summary

- **Reading**:
  - Nielsen chapter 1
  - Goodfellow et al sections 5.9, 6.1, 6.2, 8.1
- Stochastic gradient descent (SGD) and minibatch
- Classification and regression
- Sigmoid activation function and cross-entropy
- Multiple classes – Softmax
- Next lecture: multi-layer networks and hidden units