Revision sheet

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Exercise 1. Consider a prediction rule $h: \mathbb{R}^d \to \mathbb{R}^q_+$ with $h(x) = (h_1(x), ..., h_q(x))^\top$ which receives inputs $x = (x_1, ..., x_d)^\top \in \mathbb{R}^d$ and which is modeled as a feedforward neural network (NN) with equation

$$h_k(x) = \sigma_2 \left(\sum_{j=1}^{c} w_{2,k,j} \sigma_1 \left(\sum_{i=1}^{d} w_{1,j,i} x_i \right) \right)$$

for k = 1, ..., q. We consider activation functions $\sigma_1(a) = \frac{1}{1 + \exp(-a)}$ and $\sigma_2(a) = \log(1 + \exp(a))$. Parameters $c \in \mathbb{N}_+$, and $d \in \mathbb{N}_+$ are considered as known, while the weights $\{w_{\cdot,\cdot,\cdot}\}$ of the NN are unknown. To learn the unknown weights $\{w_{\cdot,\cdot,\cdot}\}$, we specify the loss function

$$\ell(w, z = (x, y)) = \frac{1}{2} \|h(x) - y\|_{2}^{2} = \frac{1}{2} \sum_{k=1}^{q} (h_{k}(x) - y_{k})^{2}$$

where z = (x, y) denotes an example, $x \in \mathbb{R}^d$ is the input vector (features), and $y = (y_1, ..., y_q)^{\top} \in \mathbb{R}^q$ is the output vector (targets).

- (1) Perform the forward pass of the back-propagation procedure to compute the activations which may be denoted as $\{a_{t,i}\}$ and outputs which may be denoted as $\{o_{t,i}\}$ at each layer t.
- (2) Perform the backward pass of the back-propagation procedure in order to compute the gradient

$$\nabla_{w}\ell\left(w,\left(x,y\right)\right) = \left(\left(\frac{\partial}{\partial w_{1,j,i}}\ell\left(w,\left(x,y\right)\right)\right)_{j=1,i=1}^{c,d}, \left(\frac{\partial}{\partial w_{2,k,j}}\ell\left(w,\left(x,y\right)\right)\right)_{k=1,j=1}^{q,c}\right)\right)$$

of the loss function $\ell(w, z)$ with respect to w for any example z = (x, y). Clearly state the steps of the procedure as well as state the quantities

$$\frac{\partial}{\partial w_{1,j,i}}\ell\left(w,\left(x,y\right)\right)$$
, and $\frac{\partial}{\partial w_{2,k,j}}\ell\left(w,\left(x,y\right)\right)$

for all k = 1, ..., q, j = 1, ..., c, and i = 1, ..., d.

Solution. I 've got T = 2 layers.

(1) Regarding the forward pass. It is

Set: Comp for i = 1, ..., d

$$o_{0,i}\left(x\right) = x_i$$

t=1: Comp

$$\alpha_{1,j}(x) = \sum_{i=1}^{d} w_{1,j,i} x_i$$

$$o_{1,j}(x) = (1 + \exp(-\alpha_{1,j}(x)))^{-1}$$

t=2: Comp

$$\alpha_{2,k}(x) = \sum_{j=1}^{c} w_{2,k,j} o_{1,j}(x)$$

$$o_{2,k}(x) = \log(1 + \exp(\alpha_{2,k}(x)))$$

Get: Comp for k = 1, ..., q

$$h_k\left(x\right) = o_{2,k}\left(x\right)$$

(2) Regarding the backward pass. It is

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\sigma_2(\xi) = \frac{\exp(\xi)}{1 + \exp(\xi)} = \sigma_1(\xi)$$

and

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\sigma_{1}\left(\xi\right) = -\frac{\exp\left(-\xi\right)}{1 + \exp\left(-\xi\right)} \frac{1}{1 + \exp\left(-\xi\right)}$$
$$= -\sigma_{1}\left(\xi\right)\left(1 - \sigma_{1}\left(\xi\right)\right)$$

t=T=2:

$$\tilde{\delta}_{T=2,k} = \frac{\mathrm{d}}{\mathrm{d}o_{T,k}} \ell_T(w, z) \frac{\mathrm{d}o_{T,k}}{\mathrm{d}\alpha_{T,k}}$$
$$= (o_{T,k} - y_k) \sigma_1(\alpha_{T,k})$$
$$= (h_k - y_k) \sigma_1(\alpha_{T,k})$$

or for k = 1, ..., q

$$\tilde{\delta}_{2,k} = (h_k - y_k) \, \sigma_1 \left(\alpha_{T,k} \right)$$

t=1:

$$\tilde{\delta}_{t=1,k} = \sum_{k=1}^{q} w_{1,k,j} \tilde{\delta}_{2,k} \left. \frac{\mathrm{d}}{\mathrm{d}\xi} \sigma_{1} \left(\xi \right) \right|_{\xi = \alpha_{j}}$$

$$= -\sigma_{1} \left(\alpha_{j} \right) \left(1 - \sigma_{1} \left(\alpha_{j} \right) \right) \left[\sum_{k=1}^{q} w_{1,k,j} \tilde{\delta}_{2,k} \right]$$

Hence

$$\frac{\mathrm{d}}{\mathrm{d}w_{2,k,j}}\ell\left(w,\left(x,y\right)\right) = \left(h_{k} - y_{k}\right)\sigma_{1}\left(\alpha_{2,k}\right)o_{1,j}\left(x\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}w_{1,j,i}}\ell\left(w,\left(x,y\right)\right) = -\sigma_{1}\left(\alpha_{j}\right)\left(1 - \sigma_{1}\left(\alpha_{j}\right)\right)\left[\sum_{k=1}^{q} w_{1,k,j}\tilde{\delta}_{2,k}\right] o_{0,i}\left(x\right)$$

Exercise 2. Consider the binary classification learning problem: Let the set of targets be $\mathcal{Y} = \{-1, +1\}$, let the set of inputs be $\mathcal{X} = \{x \in \mathbb{R}^d : \|x\|_2 \leq B\}$ for some scalar B > 0, let the prediction rule be $h_w(x) = x^\top w$, and let the loss function ℓ be

$$\ell(w, z = (x, y)) = \log\left(1 + \exp\left(-yx^{\top}w\right)\right),$$

for $x \in \mathcal{X}$, $y \in \mathcal{Y}$, and $w \in \mathcal{W}$ where $\mathcal{W} = \{w \in \mathbb{R}^d : ||w||_2 \le B\}$.

- (1) Show that the resulting learning problem is convex-Lipschitz-bounded. Specify the parameter of Lipschitzness.
- (2) Show that the above loss $\ell(w, z = (x, y))$ is $B^2/4$ smooth.

Hint:: You may use the mean value theorem which states that (under pre-assumed conditions), $f(b) - f(a) = \frac{d}{dx} f(x)|_{x=c} (b-a)$ for $a \le c \le b$.

(3) Consider a risk function $R_g(w) = \mathbb{E}_{z \sim g} (\ell(w, z = (x, y)))$ where g denotes the unknown data generating process. Assume there is a set of available examples $\mathcal{D} = \{z_i = (x_i, y_i); i = 1, ..., n\}$. Now assume that $w \in \mathbb{R}^d$. To learn w, we aim to compute $w^* \in \mathbb{R}^d$ such that

$$w^* = \operatorname*{arg\,min}_{w} \left(f\left(w \right) \right)$$

where $f(w) = R_g(w) + \frac{\lambda}{2} ||w||_2^2$.

(a) Show that the stochastic gradient descent algorithm with batch size one and with learning rate

$$\eta_t = \frac{1}{\lambda t}$$

at iteration $t \in \mathbb{N}_+$ which is used to address the learning problem under consideration has a recursion that can be written in the form

$$w^{(t+1)} = -\frac{1}{\lambda t} \sum_{j=1}^{t} v_j$$

where $\{v_j\}$ is the gradient of the loss function at certain values of w and example. Show your working.

(b) Compute the exact formula of v_j as a function of λ , t, \mathcal{D} , and $\{w^{(t)}\}$. Show your working.

Solution.

(1)

Convexity:: Note that the function $g: \mathbb{R} \to \mathbb{R}$, defined by $g(a) = \log(1 + \exp(a))$ is convex. To see this, note that

$$\frac{d^2}{da^2}g(a) = \frac{\exp(a)}{(1 + \exp(a))^2} \ge 0$$

is non-negative. The convexity of $\ell(\cdot, z)$ for all z follows as a composition of g with a linear function.

Lipschitzness:: The function $g(a) = \log(1 + \exp(a))$ is 1-Lipschitz since

$$\left| \frac{\mathrm{d}}{\mathrm{d}a} g\left(a\right) \right| = \frac{\exp\left(a\right)}{1 + \exp\left(a\right)} = \frac{1}{\exp\left(-a\right) + 1} \le 1$$

Hence because $|x|_2 \leq B$, g(a) is B-Lipschitz as a composition.

Boundness:: The norm of each hypothesis w is bounded by B according to the assumptions.

(2) Smoothness:: It is

$$\frac{d^{2}}{da^{2}}g(a) = \frac{\exp(a)}{(1 + \exp(a))^{2}}$$

$$= \frac{1}{\exp(a)(1 + \exp(-a))^{2}}$$

$$= \frac{1}{2 + \exp(a) + \exp(-a)} \le 1/4$$

Combine this with the mean value theorem, to conclude that $\frac{d}{da}g(a)$ is 1/4-Lipschitz. Hence, $\ell(\cdot, z)$ for all z is $B^2/4$ smooth.

(a) I need to minimize

$$f(w) = R_g(w) + \frac{\lambda}{2} \|w\|_2^2$$

= $E_{z \sim g} \left(\ell(w, z = (x, y)) + \frac{\lambda}{2} \|w\|_2^2 \right)$

so the online SGD has a recursion

$$w^{(t+1)} = w^{(t)} - \frac{1}{\lambda t} \left(\lambda w^{(t)} + v_t \right)$$

where

$$v_t = \frac{\mathrm{d}}{\mathrm{d}\xi} \ell \left(\xi, z^{(t)} = \left(x^{(t)}, y^{(t)} \right) \right) \Big|_{\xi = w^{(t)}}$$

and $(x^{(t)}, y^{(t)})$ is a randomly drawn example from the dataset. The recursion is

$$w^{(t+1)} = w^{(t)} - \frac{1}{\lambda t} \left(\lambda w^{(t)} + v_t \right)$$

$$= \left(1 - \frac{1}{t} \right) w^{(t)} - \frac{1}{\lambda t} v_t$$

$$= \underbrace{\frac{t-1}{t} w^{(t)} - \frac{1}{\lambda t} v_t}_{=\zeta_t}$$

$$= \frac{t-1}{t} \left(\frac{t-2}{t-1} w^{(t-1)} - \frac{1}{\lambda (t-1)} v_{t-1} \right) - \frac{1}{\lambda t} v_t$$

$$= \frac{t-2}{t-1} w^{(t-1)} - \frac{1}{\lambda t} \left(v_{t-1} + v_t \right)$$

$$= -\frac{1}{\lambda t} \sum_{j=1}^{t} v_j$$

(b) Regarding the exact formula of v_t

$$v_{t} = -\frac{\exp\left(-y^{(t)} \left(x^{(t)}\right)^{\top} w^{(t)}\right)}{1 + \exp\left(-y^{(t)} \left(x^{(t)}\right)^{\top} w^{(t)}\right)} y^{(t)} x^{(t)}$$

where $(x^{(t)}, y^{(t)})$ is a randomly drawn example from the dataset. This is because

$$\frac{\mathrm{d}}{\mathrm{d}w}\ell\left(w,z=(x,y)\right) = \frac{\mathrm{d}}{\mathrm{d}w}\log\left(1 + \exp\left(-yx^{\top}w\right)\right)$$
$$= -\frac{\exp\left(-yx^{\top}w\right)}{1 + \exp\left(-yx^{\top}w\right)}yx$$