CS480/680: Introduction to Machine Learning

Homework 1

Due: 11:59 pm, May 29, 2024, submit on LEARN.

NAME
student number

Submit your writeup in pdf and all source code in a zip file (with proper documentation). Write a script for each programming exercise so that the TA can easily run and verify your results. Make sure your code runs!
[Text in square brackets are hints that can be ignored.]

Exercise 1: Perceptron (8 pts)

Convention: All algebraic operations, when applied to a vector or matrix, are understood to be element-wise (unless otherwise stated).

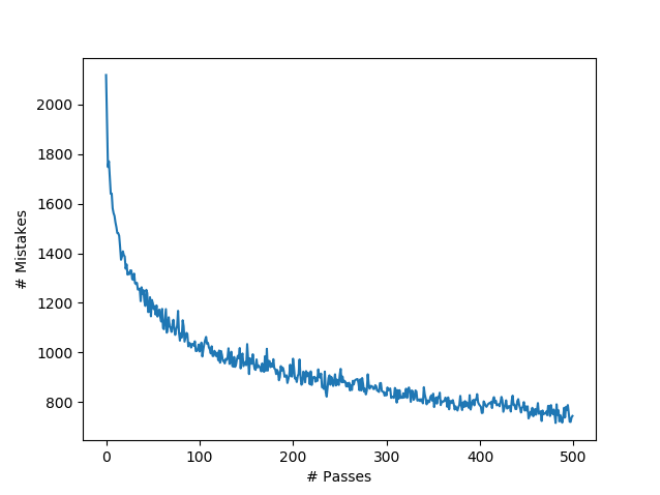
Algorithm 1: The perceptron.

Input: $X \in \mathbb{R}^{d \times n}$, $\mathbf{y} \in \{-1, 1\}^n$, $\mathbf{w} = \mathbf{0}_d$, $b = 0$, max_pass $\in \mathbb{N}$
Output: $\mathbf{w}, b, mistake$

```
for t = 1, 2, ..., max_pass do
    mistake(t) ← 0
    for i = 1, 2, ..., n do
        if y_i(⟨x_i, w⟩ + b) ≤ 0 then
            w ← w + y_i x_i                    // x_i is the i-th column of X
            b ← b + y_i
            mistake(t) ← mistake(t) + 1
```

1. (1 pt) Implement the perceptron in Algorithm 1. Your implementation should take input as $X = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$, $\mathbf{y} \in \{-1, 1\}^n$, an initialization of the hyperplane parameters $\mathbf{w} \in \mathbb{R}^d$ and $b \in \mathbb{R}$, and the maximum number of passes of the training set [suggested max_pass $= 500$]. Run your perceptron algorithm on the spambase dataset (available on course website), and plot the number of mistakes (y-axis) w.r.t. the number of passes (x-axis).

   Ans:



2. (1 pt) Using the one-vs-all reduction to implement a multiclass perceptron. You may call your binary implementation. Test your algorithm on the activity dataset (available on course website), and report your final errors on the training and test sets.

   Ans:

```
>>> One-vs-all reduction ...
Errors on the training set by one-vs-all reduction: 308 (with max_pass=50).
Errors on the test set by one-vs-all reduction: 198 (with max_pass=50).
Time cost for Ex1.2:  24.04 s.
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```
>>> One-vs-all reduction ...
Errors on the training set by one-vs-all reduction: 139 (with max_pass=500).
Errors on the test set by one-vs-all reduction: 145 (with max_pass=500).
Time cost for Ex1.2:  132.63 s.
```

3. (1 pt) Using the one-vs-one reduction to implement a multiclass perceptron. You may call your binary implementation. Test your algorithm on the activity dataset (available on course website), and report your final errors on the training and test sets.

   Ans:

```
>>> One-vs-one reduction ...
Errors on the training set by one-vs-one reduction: 121 (with max_pass=50).
Errors on the test set by one-vs-one reduction: 205 (with max_pass=50).
Time cost for Ex1.3:  12.29 s.
```

```
>>> One-vs-one reduction ...
Errors on the training set by one-vs-one reduction: 139 (with max_pass=500).
Errors on the test set by one-vs-one reduction: 152 (with max_pass=500).
Time cost for Ex1.3:  112.45 s.
```

4. (2 pts) Consider the (continuous) piece-wise function

$$f(\mathbf{w}) := \max_k f_k(\mathbf{w}), \tag{1}$$

   where each f_k is continuously differentiable. We define the derivative of f at any $\mathbf{w}$ as follows: first find (any) k such that $f(\mathbf{w}) = f_k(\mathbf{w})$, i.e. $f_k(\mathbf{w})$ achieves the maximum among all pieces; then we let $f'(\mathbf{w}) = f'_k(\mathbf{w})$. [Clearly, the index k that achieves maximum may depend on $\mathbf{w}$, the point we evaluate the derivative at.] Now consider the following problem [padding applied, $y_i \in \{\pm 1\}$]:

$$\min_{\mathbf{w}} \sum_{i=1}^{n} \max\{0, -y_i(\langle \mathbf{x}_i, \mathbf{w}\rangle)\}. \tag{2}$$

   Prove that in each iteration, the (binary) perceptron algorithm essentially picks a term from the above summation, computes the corresponding derivative (say $\mathbf{g}$), and performs a gradient update:

$$\mathbf{w} \leftarrow \mathbf{w} - \mathbf{g}. \tag{3}$$

   [You may ignore the degenerate case when $\langle \mathbf{x}_i, \mathbf{w}\rangle = 0$, and you can use the usual chain rule for our derivative.]

   Ans: We simply verify that at each iteration, say when the I_t-th term is chosen, the gradient is

$$\mathbf{g} = \begin{cases} 0, & \text{if } y_{I_t}\hat{y}_{I_t} > 0 \\ -y_{I_t}\mathbf{x}_{I_t}, & \text{if } y_{I_t}\hat{y}_{I_t} \le 0 \end{cases}, \tag{4}$$

   which follows from the fact mentioned at the beginning about the derivative of the piecewise function $f = \max_k f_k$, where we identify $f_1(\mathbf{w}) \equiv 0$ and $f_2(\mathbf{w}) = -y_i\langle \mathbf{x}_i, \mathbf{w}\rangle$.

5. (1 pt) Consider the following problem, where $y_i \in \{1, 2, \ldots, c\}$:

$$\min_{\mathbf{w}_1,\ldots,\mathbf{w}_c} \sum_{i=1}^{n} \max_{k=1,\ldots,c} \Big[\langle \mathbf{x}_i, \mathbf{w}_k\rangle - \langle \mathbf{x}_i, \mathbf{w}_{y_i}\rangle\Big]. \tag{5}$$

   Show that when $c = 2$, we reduce to the binary perceptron problem in (2). [Try to identify the weights $\mathbf{w}$, using some transformation.]

Ans: When $c = 2$, we may define $\mathbf{w} = \mathbf{w}_1 - \mathbf{w}_2$ so that

$$\max_{k=1,\dots,c} [\langle \mathbf{x}_i, \mathbf{w}_k \rangle - \langle \mathbf{x}_i, \mathbf{w}_{y_i} \rangle] = \max\{0, (2y_i - 3)\langle \mathbf{x}_i, \mathbf{w} \rangle\}, \tag{6}$$

which, up to a redefinition of the label, is exactly (2).

6. (2 pts) Based on the analogy to the binary case, develop and implement a multiclass perceptron algorithm to solve (5) directly. Run your implementation on the activity dataset (available on course website) and report the final errors on the training and test sets. [Hint: obviously, we want to predict as follows: $\hat{y} = \operatorname{argmax}_{k=1,\dots,c} \langle \mathbf{x}, \mathbf{w}_k \rangle$, i.e., the class k whose corresponding $\mathbf{w}_k$ maximizes the inner product. Explain your algorithm (e.g., through pseudo-code).]

Ans: The update is as follows:

- choose index I_t
- find

$$v = \max_{k \neq y_{I_t}} \langle \mathbf{x}_{I_t}, \mathbf{w}_k \rangle - \langle \mathbf{x}_{I_t}, \mathbf{w}_{y_{I_t}} \rangle \tag{7}$$

$$\kappa = \operatorname*{argmax}_{k \neq y_{I_t}} \langle \mathbf{x}_{I_t}, \mathbf{w}_k \rangle - \langle \mathbf{x}_{I_t}, \mathbf{w}_{y_{I_t}} \rangle, \quad \text{[break ties arbitrarily]}. \tag{8}$$

- the gradient $[\mathbf{g}_1, \dots, \mathbf{g}_c] = \mathbf{0}$ by default (i.e. no update), with the exception that if $v \geq 0$, then

$$\mathbf{g}_\kappa = \mathbf{x}_{I_t} \tag{9}$$

$$\mathbf{g}_{y_{I_t}} = -\mathbf{x}_{I_t}. \tag{10}$$

[In fact, even if we do not restrict $k \neq y_{I_t}$, the update will remain the same since when $k = y_{I_t}$, the update is effectively vacuous.]

```
>>> Ex1.6 ...
Errors on the training set by alg Ex1.6: 269 (with max_pass=50).
Errors on the test set by alg Ex1.6: 177 (with max_pass=50).
Time cost for Ex1.6:  14.51 s.
```

```
>>> Ex1.6 ...
Errors on the training set by alg Ex1.6: 129 (with max_pass=500).
Errors on the test set by alg Ex1.6: 140 (with max_pass=500).
Time cost for Ex1.6:  127.38 s.
```

Exercise 2: Generalized linear models (6 pts)

Recall that in logistic regression we assumed the *binary* label $\mathsf{Y}_i \in \{0, 1\}$ follows the Bernoulli distribution: $\Pr(\mathsf{Y}_i = 1 | \mathsf{X}_i) = p_i$, where p_i also happens to be the mean. Under the independence assumption we derived the (conditional) negative log-likelihood function:

$$-\sum_{i=1}^{n} (1 - y_i) \log(1 - p_i) + y_i \log(p_i). \tag{11}$$

Then, we parameterized the mean parameter p_i through the logit transform:

$$\log \frac{p_i}{1 - p_i} = \langle \mathbf{x}_i, \mathbf{w} \rangle + b, \quad \text{or equivalently} \quad p_i = \frac{1}{1 + \exp(-\langle \mathbf{x}_i, \mathbf{w} \rangle - b)}. \tag{12}$$

Lastly, we found the weight vector $\mathbf{w}$ and b by minimizing the negative log-likelihood function.

In the following we generalize the above idea significantly. Let the (conditional) density of Y (given $\mathsf{X} = \mathbf{x}$) be

$$p(y|\mathbf{x}) = \exp\Big[\mu(\mathbf{x}) \cdot y - \lambda(\mathbf{x})\Big] \cdot q(y), \tag{13}$$

where $\mu : \mathbb{R}^d \to \mathbb{R}$ is a function of $\mathbf{x}$ and $\lambda(\mathbf{x}) = \log \int_y \exp\big(\mu(\mathbf{x}) \cdot y\big) q(y) \mathrm{d}y$ so that $p(y|\mathbf{x})$ is properly normalized wrt y (i.e., integrate to 1). For discrete y (such as in logistic regression), replace the density with the probability mass function and the integral with sum.

As always, you need to supply sufficient derivation details to justify your final answer.

1. (1 pt) Given a dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, derive the (conditional) negative log-likelihood function of $y_1, \ldots, y_n$, assuming independence and the density in (13).

   Ans: We have

$$\sum_{i=1}^n -\mu(\mathbf{x}_i) y_i + \lambda(\mathbf{x}_i) - \log q(y_i) \tag{14}$$

2. (1 pt) Plug the usual linear parameterization

$$\mu(\mathbf{x}) = \langle \mathbf{x}, \mathbf{w} \rangle + b = \langle \mathbf{x}, \mathbf{w} \rangle \tag{15}$$

   into your (conditional) negative log-likelihood and compute the gradient of the resulting function. [Hint: you may swap differentiation with integral and your gradient may involve implicitly defined terms.]

   Ans: We have

$$\ell_n(\mathbf{w}) = \sum_{i=1}^n -y_i \mathbf{w}^\top \mathbf{x}_i + \lambda(\mathbf{w}; \mathbf{x}_i) - \log q(y_i), \tag{16}$$

   and hence

$$\nabla \ell_n(\mathbf{w}) = \sum_{i=1}^n (p_i - y_i)\mathbf{x}_i, \quad \text{where} \quad p_i = p_i(\mathbf{w}; \mathbf{x}_i) = \frac{\int_y y \exp(y \mathbf{w}^\top \mathbf{x}_i) q(y) \mathrm{d}y}{\int_y \exp(y \mathbf{w}^\top \mathbf{x}_i) q(y) \mathrm{d}y}. \tag{17}$$

3. (1 pt) Let us revisit linear regression, where

$$p(y|\mathbf{x}) = \tfrac{1}{\sqrt{2\pi}} \exp\big(-\tfrac{(y - \nu(\mathbf{x}))^2}{2}\big) \tag{18}$$

   Identify the functions $\mu(\mathbf{x})$, $\lambda(\mathbf{x})$ and $q(y)$ for the above specialization. Based on the linear parameterization in Ex 2.2, derive the negative log-likelihood and gradient. [Hint: you may simply plug into the more general result in Ex 2.2. Compare with what you already learned about linear regression to make sure both Ex 2.2 and Ex 2.3 are correct.]

   Ans: We have

$$\mu(\mathbf{x}) = \nu(\mathbf{x}) \tag{19}$$
$$\lambda(\mathbf{x}) = [\nu(\mathbf{x})]^2/2 = [\mu(\mathbf{x})]^2/2 \tag{20}$$
$$q(y) = \tfrac{1}{\sqrt{2\pi}} \exp(-y^2/2) \tag{21}$$
$$\ell_n(\mathbf{w}) = \sum_{i=1}^n -y_i \mathbf{w}^\top \mathbf{x}_i + \lambda(\mathbf{w}; \mathbf{x}_i) - \log q(y_i) \tag{22}$$
$$\nabla \ell_n(\mathbf{w}) = \sum_{i=1}^n (p_i - y_i)\mathbf{x}_i, \quad \text{where} \quad p_i = \mu(\mathbf{x}_i) \tag{23}$$

4. (1 pt) Let us revisit logistic regression, where

$$\Pr(\mathsf{Y} = y|\mathbf{x}) = [\nu(\mathbf{x})]^y [1 - \nu(\mathbf{x})]^{1-y}, \quad \text{where} \quad y \in \{0, 1\}. \tag{24}$$

Identify the functions $\mu(\mathbf{x})$, $\lambda(\mathbf{x})$ and $q(y)$ for the above specialization. Based on the linear parameterization in Ex 2.2, derive the negative log-likelihood and gradient. [Hint: Compare with what you already learned about logistic regression.]

Ans: We have

$$\mu(\mathbf{x}) = \log \frac{\nu(\mathbf{x})}{1-\nu(\mathbf{x})} \tag{25}$$

$$\lambda(\mathbf{x}) = -\log(1-\nu(\mathbf{x})) = \mu(\mathbf{x}) + \log\left(1+\exp(-\mu(\mathbf{x}))\right) \tag{26}$$

$$q(y) = 1 \tag{27}$$

$$\ell_n(\mathbf{w}) = \sum_{i=1}^n -y_i \mathbf{w}^\top \mathbf{x}_i + \lambda(\mathbf{w}; \mathbf{x}_i) - \log q(y_i) \tag{28}$$

$$\nabla \ell_n(\mathbf{w}) = \sum_{i=1}^n (p_i - y_i)\mathbf{x}_i, \quad \text{where} \quad p_i = \tfrac{1}{1+\exp(-\mu(\mathbf{x}_i))} \tag{29}$$

5. (2 pts) Now let us tackle something new. Let

$$\Pr(\mathsf{Y} = y|\mathbf{x}) = \frac{[\nu(\mathbf{x})]^y}{y!}\exp(-\nu(\mathbf{x})), \quad \text{where} \quad y = 0, 1, 2, \ldots. \tag{30}$$

Identify the functions $\mu(\mathbf{x})$, $\lambda(\mathbf{x})$ and $q(y)$ for the above specialization. Based on the linear parameterization in Ex 2.2, derive the negative log-likelihood and gradient. [Hint: Y here follows the Poisson distribution, which is useful for modeling integer-valued events, e.g. the number of customers at a given time.]

Ans: We have

$$\mu(\mathbf{x}) = \log \nu(\mathbf{x}) \tag{31}$$

$$\lambda(\mathbf{x}) = \nu(\mathbf{x}) = \exp(\mu(\mathbf{x})) \tag{32}$$

$$q(y) = 1/y! \tag{33}$$

$$\ell_n(\mathbf{w}) = \sum_{i=1}^n -y_i \mathbf{w}^\top \mathbf{x}_i + \lambda(\mathbf{w}; \mathbf{x}_i) - \log q(y_i) \tag{34}$$

$$\nabla \ell_n(\mathbf{w}) = \sum_{i=1}^n (p_i - y_i)\mathbf{x}_i, \quad \text{where} \quad p_i = \exp(\mu(\mathbf{x}_i)) \tag{35}$$

Exercise 3: Ordinal regression (4 pts)

In many applications, the "labels" have an inherent order. For example, the letter grade A is preferred to B, which is preferred to C, etc. More generally, consider c ordinal labels $1, 2, \ldots, c$, where we prefer label k than $k+1$, for each $k = 1, \ldots, c-1$. [The preference is transitive, i.e. any "smaller" label is preferred than a "larger" label.]

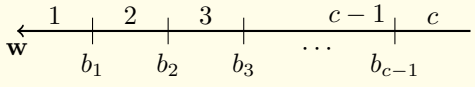
1. (2 pts) Let us consider $c-1$ *parallel* hyperplanes $H_k := \{\mathbf{x} : \langle \mathbf{x}, \mathbf{w}\rangle + b_k = 0\}$, which partition our space into c rectangular regions. We define our prediction as

$$\hat{y} \le k \iff \langle \mathbf{x}, \mathbf{w}\rangle + b_k > 0, \tag{36}$$

or more explicitly,

$$\hat{y} = k \iff [\langle \mathbf{x}, \mathbf{w}\rangle + b_k > 0 \text{ and } \langle \mathbf{x}, \mathbf{w}\rangle + b_{k-1} \le 0], \tag{37}$$

where $b_0 := -\infty$ and $b_c := \infty$.



The ordering in the labels is now respected, if we constrain $b_1 \le b_2 \le \cdots \le b_{c-1}$:

$$\hat{y} \le k \implies \hat{y} \le l, \quad \forall\, l \ge k. \tag{38}$$

We learn the weights $\mathbf{w}$ and $b_1, \ldots, b_{c-1}$ by reducing to a sequence of (coupled) binary classifications:

$$\min_{\mathbf{w}, b_1 \le b_2 \le \cdots \le b_{c-1}} \frac{\lambda}{2}\|\mathbf{w}\|_2^2 + \sum_{k=1}^{c-1}\sum_{i=1}^{n} \max\{0, 1 - (\llbracket y_i = k \rrbracket - \llbracket y_i = k+1 \rrbracket)(\langle \mathbf{x}_i, \mathbf{w}\rangle + b_k)\}, \tag{39}$$

where recall that $\llbracket A \rrbracket$ is 1 if A is true and 0 otherwise. It is clear that when $c = 2$, the above reduces to the familiar soft-margin SVM. Derive the Lagrangian dual of (39). [If it helps, you may ignore the constraint $b_1 \le \ldots \le b_{c-1}$.]

Ans: We derive the dual as follows:

$$\min_{\mathbf{w}, \mathbf{b}} \max_{\mathbf{1} \ge \boldsymbol{\alpha} \ge \mathbf{0}, \boldsymbol{\beta} \ge \mathbf{0}} \frac{\lambda}{2}\|\mathbf{w}\|_2^2 + \sum_{k=1}^{c-1} \left\{ (b_k - b_{k+1})\beta_k + \sum_{i=1}^{n} \alpha_{ki} \left[1 - (\llbracket y_i = k \rrbracket - \llbracket y_i = k+1 \rrbracket)(\langle \mathbf{x}_i, \mathbf{w}\rangle + b_k)\right] \right\}. \tag{40}$$

Take derivative w.r.t. $\mathbf{w}$ and $\mathbf{b}$ we obtain

$$\mathbf{w} = \frac{1}{\lambda}\sum_{k=1}^{c-1}\sum_{i=1}^{n} \alpha_{ki}(\llbracket y_i = k \rrbracket - \llbracket y_i = k+1 \rrbracket)\mathbf{x}_i \tag{41}$$

$$\beta_k - \beta_{k-1} - \sum_{i=1}^{n} \alpha_{ki}(\llbracket y_i = k \rrbracket - \llbracket y_i = k+1 \rrbracket) = 0. \tag{42}$$

Plug back in and negate the sign we obtain

$$\min_{\mathbf{1} \ge \boldsymbol{\alpha} \ge \mathbf{0}, \boldsymbol{\beta} \ge \mathbf{0}} \frac{\lambda}{2}\|\mathbf{w}\|_2^2 - \sum_{k=1}^{c-1}\sum_{i=1}^{n} \alpha_{ki} \tag{43}$$

$$\text{s.t. } \beta_k - \beta_{k-1} - \sum_{i=1}^{n} \alpha_{ki}(\llbracket y_i = k \rrbracket - \llbracket y_i = k+1 \rrbracket) = 0, \quad k = 1, \ldots, c-1, \tag{44}$$

where $\mathbf{w}$ is given in (41) and by convention $\beta_0 = 0$. Using telescoping we may eliminate $\boldsymbol{\beta}$, and arrive at the final dual problem:

$$\min_{\mathbf{1} \ge \boldsymbol{\alpha} \ge \mathbf{0}} \frac{1}{2\lambda}\left\| \sum_{k=1}^{c-1}\sum_{i=1}^{n} \alpha_{ki}(\llbracket y_i = k \rrbracket - \llbracket y_i = k+1 \rrbracket)\mathbf{x}_i \right\|_2^2 - \sum_{k=1}^{c-1}\sum_{i=1}^{n} \alpha_{ki} \tag{45}$$

$$\text{s.t. } \sum_{\kappa=1}^{k}\sum_{i=1}^{n} \alpha_{ki}(\llbracket y_i = k \rrbracket - \llbracket y_i = k+1 \rrbracket) \ge 0, \quad \forall k = 1, \ldots, c-1. \tag{46}$$

2. (2 pts) In the previous formulation, to learn b_k, essentially we take class k as positive and class $k+1$ as negative. Can you find a "better" alternative? Write down the formulation. [Hint: it would be similar to (39).]

Ans: We can use all labels smaller than k as positive and all labels larger than $k+1$ as negatives to learn $(\mathbf{w}_k, b_k)$:

$$\min_{\mathbf{w}, b_1 \le b_2 \le \cdots \le b_{c-1}} \frac{\lambda}{2}\|\mathbf{w}\|_2^2 + \sum_{k=1}^{c-1}\sum_{i=1}^{n} \max\{0, 1 - (\llbracket y_i \le k \rrbracket - \llbracket y_i \ge k+1 \rrbracket)(\langle \mathbf{x}_i, \mathbf{w}\rangle + b_k)\}. \tag{47}$$

[Its dual problem is exactly (45) where we change $\llbracket y_i = k \rrbracket$ to $\llbracket y_i \le k \rrbracket$ and $\llbracket y_i = k+1 \rrbracket$ to $\llbracket y_i \ge k+1 \rrbracket$, respectively.]