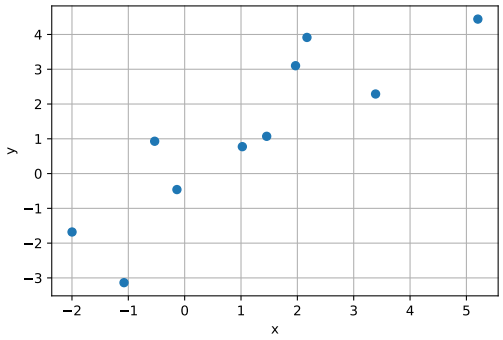
DS-GA-1003: Machine Learning (Spring 2021)

Final Exam (May 13 – May 14)

- You should finish the exam within **2 hours** once it is started and submit on Gradescope by **5:00pm EST on May 14**.
- You can refer to textbooks, lecture slides, and notes. However, searching answers online and collaboration are not allowed.
- You can write your solution either directly on the this sheet or on a separate sheet.
- Please leave enough time to upload your solution to Gradescope. You can submit it as a PDF file or any image format accepted by Gradescope. Please make sure the writings are legible.
- We suggest you save a timestamp of your start time, so that if you failed to submit in time (we hope not!), you can send us the answer sheet by email with the start and end timestamps.

Question	Points	Score
Bayesian methods	14	
Multiclass	8	
Trees	12	
Boosting	9	
Neural networks	10	
Latent variable models	13	
Total:	66	

1. **Bayesian methods.** Your are given the following dataset of N pairs of scalar real values $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$:



You would like to learn to predict y given x. Since you have little data you think it would be best to fit a simple model, yet data are not perfectly regular, so you settle for a Gaussian probabilistic conditional model with a linear predictor:

$$p(y|x,w) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(y-wx)^2} \text{ parametrized by } w \in \mathbb{R}.$$

Before seeing any data, an expert had told you that in this problem it can basically go two ways, in half of the cases y is typically equal to x or y is typically equal to $-x$. You interpret this information by using a binary prior on w:

$$p(w) = \begin{cases} 1/2 & \text{if } w = 1 \text{ or } w = -1 \\ 0 & \text{otherwise} \end{cases}.$$

(a) (2 points) Give the mathematical expression of the prior predictive function $y \mapsto p(y|x)$ describing your belief on y given a value of x taking only the probabilitic model into account (and not the data $\mathcal{D}$).

Solution

$$p(y|x) = \sum_w p(y|w,x)p(w) = \frac{1}{2\sqrt{2\pi}} e^{-\frac{1}{2}(y-x)^2} + \frac{1}{2\sqrt{2\pi}} e^{-\frac{1}{2}(y+x)^2}$$

(guide: 2pts for the expression)

(b) (2 points) Assuming $x = 2$, sketch the graph of the prior predictive function $y \mapsto p(y|x)$ for $y \in [-10, 10]$ (you should note that it is a Gaussian mixture).

Solution

Mixture of Gaussian with two equal components centered around -2 and 2.

(c) (2 points) You now consider the data $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$. Give the mathematical expression of the likelihood of the entire dataset $L(w, \mathcal{D})$ as a function of the likelihood per sample $p(y_i|w, x_i)$. Which assumption are you implicitly making?

Solution

$$L(w, \mathcal{D}) = \prod_{i=1}^{N} p(y_i|w, x_i)$$

Assuming that the data points are i.i.d.

(guide: 2pts for sketch)

(d) (4 points) Recall the definition of the posterior $p(w|\mathcal{D})$ as a function of $L(w, \mathcal{D})$ and $p(w)$ up to a multiplicative constant that is independent of w. Give the expression of $p(w|\mathcal{D})$ for the model considered here (Gaussian probabilistic conditional model and binary prior).

Solution

$$p(w|\mathcal{D}) \propto L(w, \mathcal{D})p(w) \propto \prod_{i=1}^{N} p(y_i|w, x_i)p(w) = \begin{cases} \frac{1}{2}\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(y_i - x_i)^2} & \text{if } w = 1 \\ \frac{1}{2}\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(y_i + x_i)^2} & \text{if } w = -1 \\ 0 & \text{otherwise} \end{cases}$$

(guide: 4pts for the expression)

(e) (2 points) Knowing that $\sum_{i=1}^{N}(y_i + x_i)^2 = 229.4$ and $\sum_{i=1}^{N}(y_i - x_i)^2 = 12.9$, what is $\hat{w}_{\text{MAP}}$, the maximum a posteriori estimate of w, and why?

Solution

the density at the previsous question is maximum for $w = 1$, hence it is the MAP.

(guide: 2pts for the answer)

(f) (2 points) Assume now that we are fixing w to $\hat{w}_{\text{MAP}}$. We draw a new value of x. We want to reduce the predictive function $y \mapsto p(y|x, \hat{w}_{\text{MAP}})$ to a point estimate, meaning that we want to use a single value $\hat{y}$ as prediction instead of the full distribution. How would you proceed and what would be the value of $\hat{y}$ you would choose as a function of $\hat{w}_{\text{MAP}}$ and x?

Solution

$y \mapsto p(y|x, \hat{w}_{\text{MAP}})$ is Gaussian, choosing a max or a mean are two possible strategies that would yield the same outcome $\hat{y} = \hat{w}_{\text{MAP}} x$.

(guide: 1pt for method and 1pt for $y_h at$)

2. **Multiclass loss function.** Consider a multiclass classification problem with input $x \in \mathcal{X}$ and output $y \in \mathcal{Y}$ where $\mathcal{Y} = \{1, \ldots, K\}$. Let $\varphi : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}^d$ be the feature map. Alice proposed to reduce the multilcass classification problem to binary classification in the following way. First, map each example (x, y) to $K - 1$ examples: for each $k \in \mathcal{Y} \setminus \{y\}$, create a new binary classification example where the input is

$$\varphi(x, y) - \varphi(x, k)$$

and the output is $z_k = +1$.

(a) (3 points) Suppose we use hinge loss for the binary classification problem. Write down the loss function $\ell(x, y, w)$ of a single example (x, y) where $w \in \mathbb{R}^d$ denotes the weight vector. Note that you need to first map (x, y) to binary examples then sum the hinge loss of each binary example.

Solution

$$\ell(x, y, w) = \sum_{k \in \mathcal{Y} \setminus \{y\}} \max(0, 1 - w \cdot (\varphi(x, y) - \varphi(x, k)))$$

(guide: 3pts for the function)

(b) (2 points) Given the binary classifier w, how would you predict the multiclass label for a test example x? Write an expression for the prediction $\hat{y}$.

Solution

$$\hat{y} = \arg\max_{y \in \mathcal{Y}} w \cdot \varphi(x, y)$$

(c) (3 points) Recall the generalized hinge loss for multiclass classification:

$$\ell_{\text{hinge}}(x, y, w) = \max_{y' \in \mathcal{Y}} \mathbb{I}[y \neq y'] - w \cdot (\varphi(x, y) - \varphi(x, y')),$$

where $\mathbb{I}(\cdot)$ is the indicator function. Let the groundtruth label be $y = 3$ and the total number of classes be $K = 4$. In which of the following cases would $\ell(x, y, w) = \ell_{\text{hinge}}(x, y, w)$? **Select all that apply.**

	$w \cdot \varphi(x, 3)$	$w \cdot \varphi(x, 1)$	$w \cdot \varphi(x, 2)$	$w \cdot \varphi(x, 4)$
A	3.25	2.82	1.20	1.74
B	3.25	2.82	3.11	4.60
C	3.25	2.10	0.81	1.93

Solution

A, C

(guide: 3pts for all correct; 1.5 for partial correct)

3. **Decision trees.** Consider the following dataset with input $x \in \mathbb{R}^3$ and $y \in \{0, 1\}$. Both x_i and y are binary random variables.

x_1	x_2	x_3	y
0	0	0	0
0	0	1	1
0	1	0	1
1	1	1	0

You will use *Gini index* as the impurity measure to construct a decision tree.

(a) Compute the weighted average of node impurities when splitting on each of the three features. Note that for each feature, since the value is binary, there is only one way to split. Your final answer should be a real number.

i. (2 points) Split on x_1

Solution

$$\frac{3}{4} \times (\frac{2}{3} \times \frac{1}{3} + \frac{1}{3} \times \frac{2}{3}) + \frac{1}{4} \times 0 = \frac{1}{3}$$

(guide: 2pts for the split)

ii. (2 points) Split on x_2
Solution

$$\frac{1}{2} \times (\frac{1}{2} \times \frac{1}{2} + \frac{1}{2} \times \frac{1}{2}) + \frac{1}{2} \times (\frac{1}{2} \times \frac{1}{2} + \frac{1}{2} \times \frac{1}{2}) = \frac{1}{2}$$

(guide: 2pts for the split)

iii. (2 points) Split on x_3
Solution
Same as x_2:

$$\frac{1}{2}$$

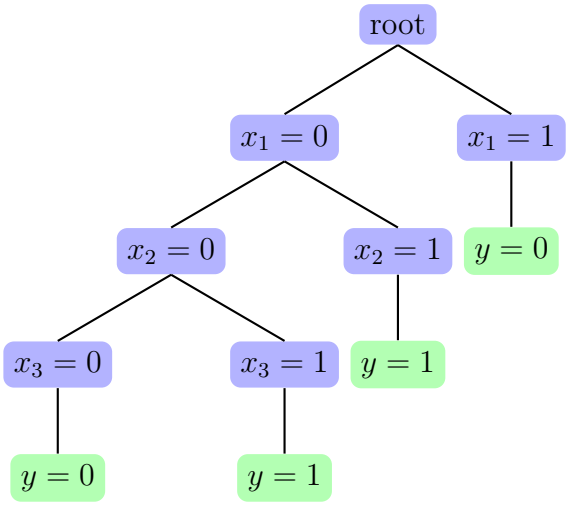
(guide: 2pts for the split)

(b) (3 points) Draw the full decision tree and write the prediction for each leaf node. You can split ties arbitrarily.

Solution

First split on x_1, then on either x_2 or x_3.

(guide: 3pts for all correct, each split from x_1 to x_3 takes 1pt.)



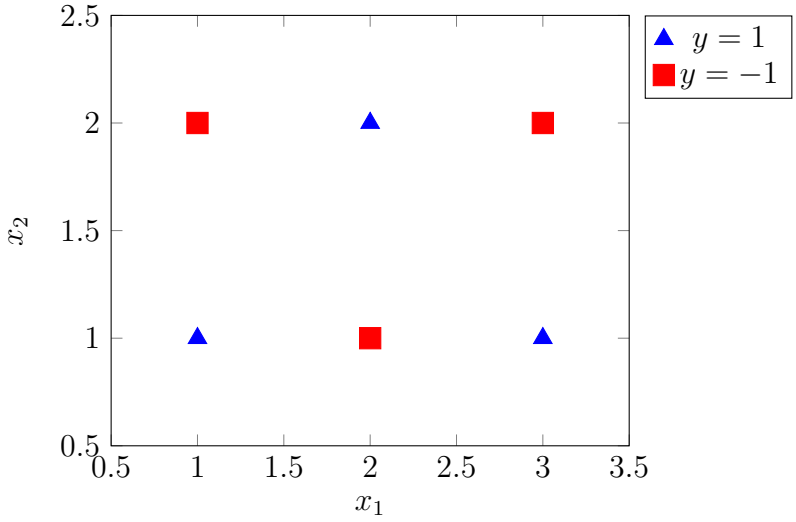
(c) (3 points) Is the above decision tree contructed using the greedy approach optimal (i.e the minimum depth tree with zero training error)? If yes, explain in one sentence; if not, draw a decision tree with smaller depth and zero training error.

Solution

Note that y is an xor function of x_2 and x_3, and x_1 is irrelevant. So we can build a tree with depth 2.

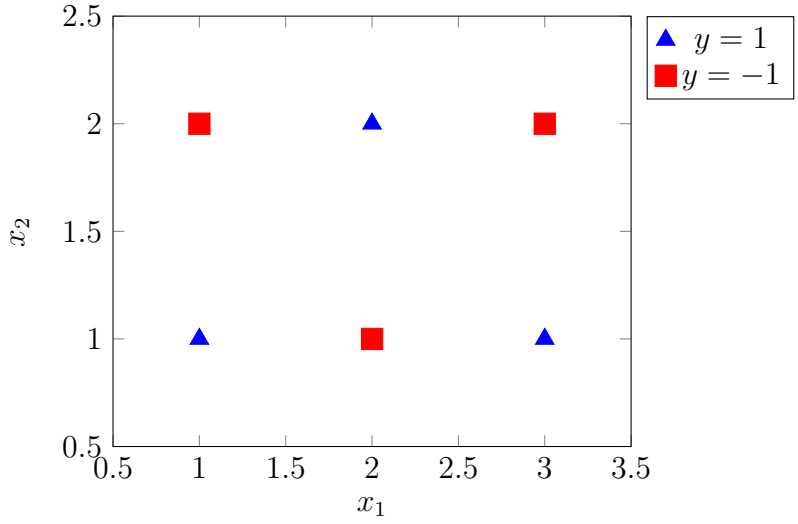
(guide: 1pt for answering "no", 2pts for drawing the tree with depth 2.)

4. **Adaboost.** Consider the following binary classification dataset:



Alice plans to use Adaboost to solve the problem but she is not sure which base/weak classifier to use. For each of the base classifier choice below, (1) explain if Adaboost (using the base classifier) can reach 100% accuracy on the dataset; (2) if yes, draw the decision boundary in the first iteration and circle the points whose weights will increase in the next iteration.

(a) (3 points) Linear classifier: $f(x) = w_1x_1 + w_2x_2 + b$

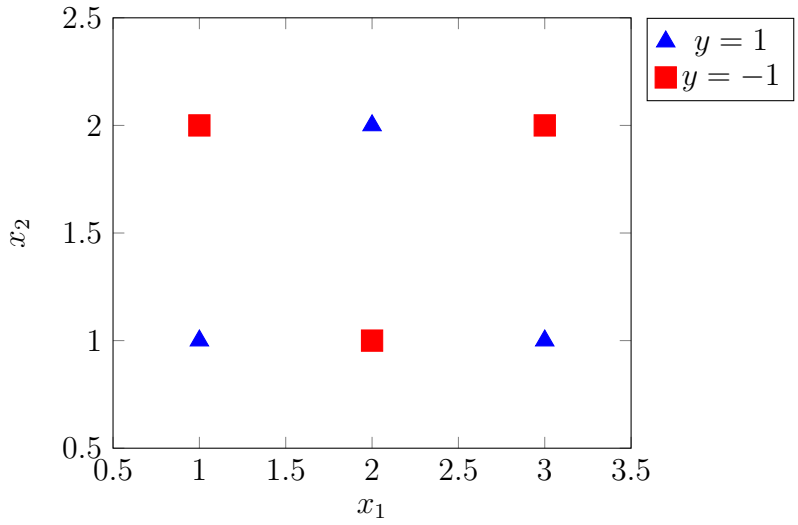


Solution

No. Boosted classifier is still linear.

(guide: 1.5pt for answering "no", 1.5pt for explanation.)

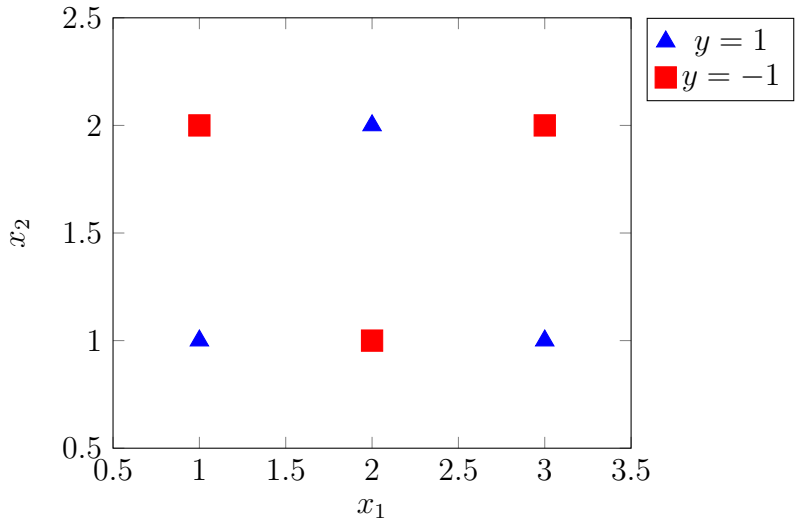
(b) (3 points) Decision stump: depth-1 decision tree



Solution

No. The base classifier cannot reach above 50% accuracy.
(guide: 1.5pt for answering "no", 1.5pt for explanation.)

(c) (3 points) Quadratic classifier: $f(x) = w_1 x_1^2 + w_2 x_2^2 + w_3 x_1 x_2 + b$



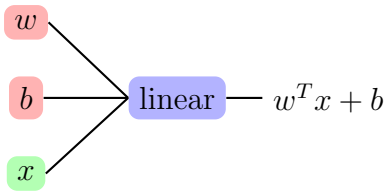
Solution

Yes. Circle any two red (or blue) dots, the one red (or blue) point left will have increased weights.

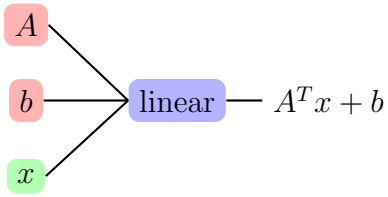
(guide: 1.5pt for answering "yes", 1.5pt drawing.)

5. **Neural networks.** Consider the following types of nodes in a computation graph. Blue, red, and green nodes represents functions, parameters, and inputs respectively. You do *not* need to color the nodes when drawing computation graphs though.

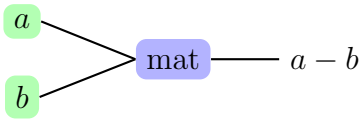
Linear node:



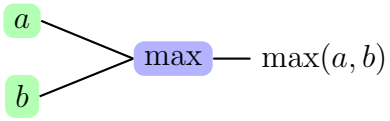
Matrix multiplication node:



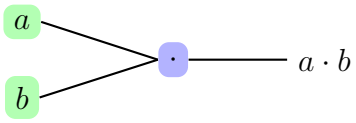
Subtraction node:



Max node:

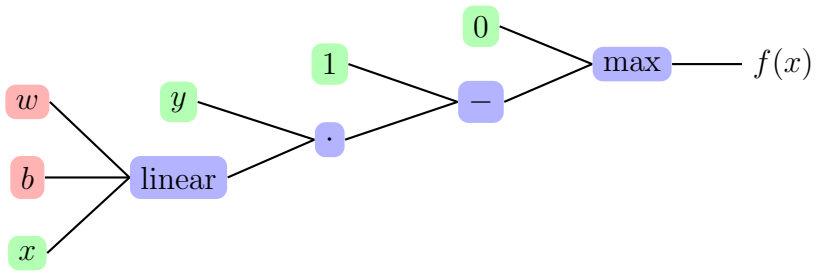


Dot node:



Note that if the input are vectors, the max node outputs the maximum value of the two vectors for each coordinate.

(a) (2 points) Consider the following computation graph:



Give an expression for $f(x, y)$.

Solution

$$f(x, y) = \max(1 - y(w^T x + b), 0)$$

(guide: 2pts for the expression.)

(b) (1 point) Let x and y denote the input and label for a binary classification task. What is the name of the loss function given by the function f above?

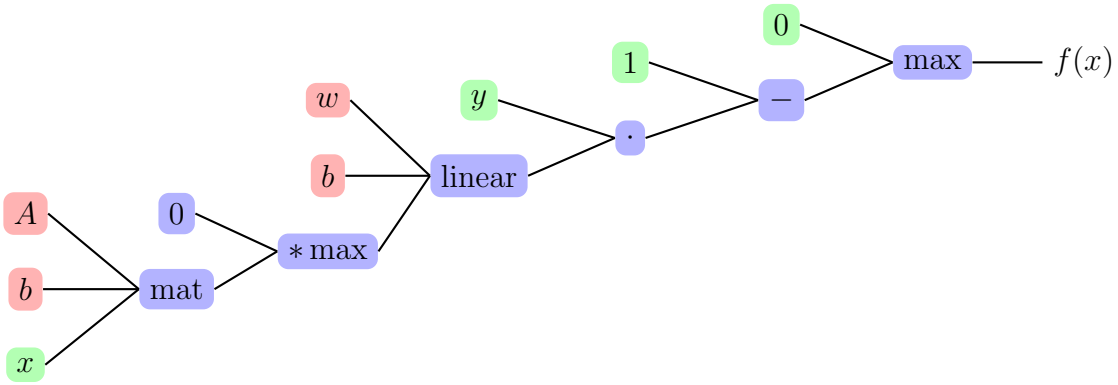
Solution

Hinge loss.

(guide: 1pt for the answer.)

(c) (4 points) Modify the above computation graph to compute the hinge loss of a two-layer (one hidden layer) neural network with ReLU activation, and circle the node corresponding to the activation function. Please only use the computation nodes given above.

Solution



The max node with $*$ is the activation node.

(guide: 3pts for the plot, 1pt for the circle.)

(d) (3 points) Give an expression for the output of your computation graph in the previous question.

Solution

$$f(x, y) = \max(1 - y(w \cdot \max(0, A^T x + b) + b'), 0)$$

(guide: 3pts for the expression.)

6. **Gaussian mixture models.** Consider a Gaussian mixture model with two mixture components:

$$z \sim \text{categorical}(\pi_1, \pi_2),$$
$$x \mid z = i \sim \mathcal{N}(\mu_i, \sigma_i).$$

where $\mu_i \in \mathbb{R}$. Suppose we know the true value of the following parameters:

$$\sigma_1 = \sigma_2 = 1,$$
$$\pi_1 = \pi_2 = 0.5.$$

Now we want to estimate μ_i given some observed data using the EM algorithm.

(a) Suppose at initialization, we have $\hat{\mu}_1 = \hat{\mu}_2 = 0$.

i. (2 points) What is the posterior of z estimated in the E-step? Give expressions for $p(z = 1 \mid x)$ and $p(z = 2 \mid x)$. Your final answer should be a real number.
Solution
$p(z = 1 \mid x) = p(z = 2 \mid x) = 0.5$
(guide: 2pts for the answer.)

ii. (3 points) What is the updated value of $\hat{\mu}_1$ and $\hat{\mu}_2$ in the M-step? You can assume that we have infinite data and your expression can contain μ_1 and μ_2.
Solution
$\hat{\mu}_1 = \hat{\mu}_2 = \frac{\mu_1+\mu_2}{2}$
(guide: 3pts for the answer.)

iii. (2 points) After the update, the marginal likelihood of the data will (You can assume that the updated values are different from the initialization)

A. increase

B. decrease

C. increase or decrease

Solution

A

(guide: 2pts for the answer.)

iv. (2 points) What is the value of $\hat{\mu}_1$ and $\hat{\mu}_2$ at convergence (i.e. the marginal likelihood no longer changes)?

Solution

It converges after one EM-step, i.e. $\hat{\mu}_1 = \hat{\mu}_2 = \frac{\mu_1+\mu_2}{2}$.

(guide: 2pts for the answer.)

(b) (2 points) Given the above result, suggest a better initialization strategy.

Solution

There are many options, e.g. pick any two random examples. The high-level principle is to pick centers that are far away from each others.

(guide: 2pts for the answer.)

(c) (2 points) Recall that in the EM algorithm, we need to decide the number of components beforehand. Suppose we try to estimate *three* components given data generated by a Gaussian mixture of *two* components. The marginal likelihood is more likely to

A. increase

B. decrease

Solution

A

(guide: 2pts for the answer.)

Congratulations! You have reached the end of the exam.