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4:00pm-5:50pm.
Wednesday, 16 Feb 2022 (or Saturday, 19 Feb 2022).

State your assumptions and reasoning.
No credit without reasoning.
Show all work on these pages.

Name: _____

Signature: _____

ID#: _____
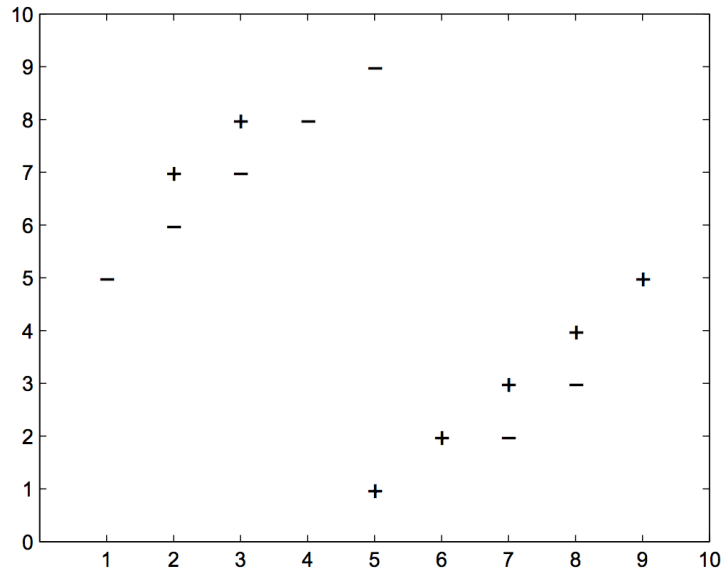
Problem 1   _____ / 25
Problem 2   _____ / 40
Problem 3   _____ / 25
Problem 4   _____ / 15
BONUS   _____ / 5 bonus points

Total   _____ / 105 points + 5 bonus points

1. **ML basics** (25 points).

(a) (5 points) Consider a k-nearest neighbors binary classifier which assigns the class of a test point to be the class of the majority of the k-nearest neighbors, according to a Euclidean distance metric. Using the data set shown above to train the classifier and choosing $k = 5$, what is the classification error on the training set? Assume that a point can be its own neighbor.

Answer as a decimal with 4 significant figures, e.g. (6.051, 0.1230, 1.234e+7) or a fraction.

solution: 0.2857

(b) (7 points) Assume we have a training and test set drawn from the same distribution, and we would like to classify points in the test set using a k-nearest neighbors classifier.

  i. (3 points) In order to minimize the classification error on this test set, we should always choose the value of k which minimizes the training set error.
     Select one:
       A. True
       B. False
     solution: B

  ii. (4 points) Consider two methods for optimizing the hyperparameters.
      - **Method 1** chooses the hyperparameters that minimize the training set error.
      - **Method 2** splits the data into training and validation sets, and chooses the hyperparameters that minimize the validation error.

2

Which method is better? Justify with no more than 3 sentences. **Select one:**

    A. Method 1

    B. Method 2

solution: B

(c) (5 points) Please select all true statements about k-nearest neighbors:

(Note: Justification is not necessary, but may result in partial credit if the answer is incorrect.)

Select all that apply:

    A Increasing k will generally result in a smoother decision boundary

    B Icreasing k will generally reduce the impact of noise or outliers in the data.

    C Increasing k increases the likelihood of overfitting the data increases.

    D It is possible to use cross-validation to select the value of k.

    E We should never select the k that minimizes the error on the validation dataset.

    F None of the above.

Solution: ABD

(d) (8 points) Consider a classifier trained till convergence on some training data D^{train}, and tested on a separate test set D^{test}. You evaluate the test error, and find that it is very high. You then compute the training error and find that it is close to 0.

    i. (3 points) Has this classifier (1) underfit, (2) reasonably fit, or (3) overfit the data?

    Solution: overfitting

    ii. (5 points) Which of the following are expected to help improve this classifier? (Note: Justification is not necessary, but may result in partial credit if the answer is incorrect.)

    Select all that apply:

A. Increase the training data size.

B. Decrease the training data size.

C. Increase model complexity.

D. Decrease model complexity.

E. Train on a combination of D^{train} and D^{test} and test on D^{test}.

F. Conclude that Machine Learning does not work.

Solution: AD

2. **Detecting signature forgery using similarity network** (40 points)

Bank of Westwood has been receiving many complaints from its clients about their signatures being forged. In order to address this problem, the bank has decided to hire you for designing a machine learning system for detecting signature forgery. You have learned about the similarity network recently and want to use it for this problem.

A similarity network is a Fully Connected Feedforward network that accepts distinct inputs but share the same weights. To be precise, $\{(\mathbf{x}^{(i)}, \hat{\mathbf{x}}^{(i)}), y^{(i)}\}$ constitutes the ith training example, where $(\mathbf{x}^{(i)} \in \mathbb{R}^d, \hat{\mathbf{x}}^{(i)} \in \mathbb{R}^d)$ represents the ith pair of single input example and $y^{(i)} \in \{+1, -1\}$ is the output label for the ith pair. For this problem,

- If the ith pair of input $(\mathbf{x}^{(i)}, \hat{\mathbf{x}}^{(i)})$ is composed of signature images both of which are genuine, then the label for the ith example is $+1$ ($y^{(i)} = +1$).

- If the ith pair of input $(\mathbf{x}^{(i)}, \hat{\mathbf{x}}^{(i)})$ is composed of signature images both of which are forged, then the label for the ith example is -1 ($y^{(i)} = -1$).

- If the ith pair of input $(\mathbf{x}^{(i)}, \hat{\mathbf{x}}^{(i)})$ is composed of signature images one of which is genuine and the other is forged, then the label for the ith example is -1 ($y^{(i)} = -1$).

The architecture of the similarity network is given below:

$$\mathbf{h}_1 = \texttt{ReLU}(\mathbf{W}_1\mathbf{x})$$
$$\hat{\mathbf{h}}_1 = \texttt{ReLU}(\mathbf{W}_1\hat{\mathbf{x}})$$
$$\mathbf{z} = \mathbf{W}_2\mathbf{h}_1$$
$$\hat{\mathbf{z}} = \mathbf{W}_2\hat{\mathbf{h}}_1$$
$$s = \cos\langle \mathbf{z}, \hat{\mathbf{z}} \rangle = \frac{\mathbf{z}^T\hat{\mathbf{z}}}{\|\mathbf{z}\|_2\|\hat{\mathbf{z}}\|_2}$$
$$\mathcal{L} = -y \cdot s$$

(a) (30 points) Having defined the architecture of the similarity network, you are now ready to learn the parameters of the network using stochastic gradient descent. The main ingredient of the gradient descent algorithms are the gradients. In the following parts, we will be walking you through the gradient computation process. To aid the gradient computations, we have drawn out the computational graph for you below. You may directly use any results derived in class.
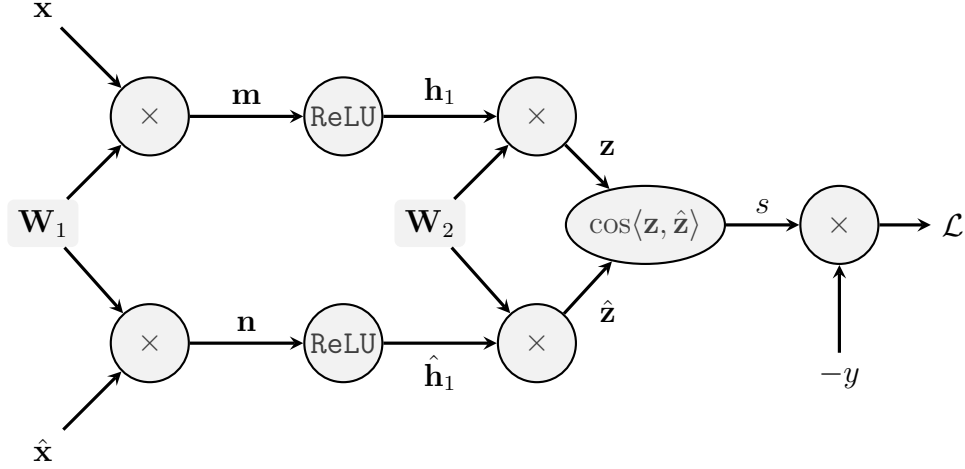
Figure 1: Computational graph of the similarity network

i. (10 points) Compute $\nabla_{\mathbf{z}}\mathcal{L}$ and $\nabla_{\hat{\mathbf{z}}}\mathcal{L}$ and denote them as $\delta_{\mathbf{z}}$ and $\delta_{\hat{\mathbf{z}}}$ respectively. For all the following parts, you can use $\delta_{\mathbf{z}}$ and $\delta_{\hat{\mathbf{z}}}$ to refer to $\nabla_{\mathbf{z}}\mathcal{L}$ and $\nabla_{\hat{\mathbf{z}}}\mathcal{L}$ respectively.

Hint: Recall the derivative quotient rule for scalars:

$$\frac{d}{dz}\left(\frac{f(z)}{g(z)}\right) = \frac{f'(z)g(z) - g'(z)f(z)}{g(z)^2}$$

for $f'(z) = \frac{df(z)}{dz}$ and $g'(z) = \frac{dg(z)}{dz}$.

Solution: By chain rule,

$$\nabla_{\mathbf{z}}\mathcal{L} = -y\frac{\partial s}{\partial \mathbf{z}}$$

$$\nabla_{\hat{\mathbf{z}}}\mathcal{L} = -y\frac{\partial s}{\partial \hat{\mathbf{z}}}.$$

Using quotient rule for multivariate derivatives, we have

$$\frac{\partial s}{\partial \mathbf{z}} = \frac{(\|\mathbf{z}\|_2\|\hat{\mathbf{z}}\|_2)\hat{\mathbf{z}} - (\mathbf{z}^T\hat{\mathbf{z}})(\frac{\|\hat{\mathbf{z}}\|_2}{\|\mathbf{z}\|_2})\mathbf{z}}{\|\mathbf{z}\|_2^2\|\hat{\mathbf{z}}\|_2^2}$$

$$\frac{\partial s}{\partial \hat{\mathbf{z}}} = \frac{(\|\mathbf{z}\|_2\|\hat{\mathbf{z}}\|_2)\mathbf{z} - (\mathbf{z}^T\hat{\mathbf{z}})(\frac{\|\mathbf{z}\|_2}{\|\hat{\mathbf{z}}\|_2})\hat{\mathbf{z}}}{\|\mathbf{z}\|_2^2\|\hat{\mathbf{z}}\|_2^2}.$$

Putting it all together, we have

$$\delta_{\mathbf{z}} = -y \cdot \frac{(\|\mathbf{z}\|_2\|\hat{\mathbf{z}}\|_2)\hat{\mathbf{z}} - (\mathbf{z}^T\hat{\mathbf{z}})(\frac{\|\hat{\mathbf{z}}\|_2}{\|\mathbf{z}\|_2})\mathbf{z}}{\|\mathbf{z}\|_2^2\|\hat{\mathbf{z}}\|_2^2}$$

$$\delta_{\hat{\mathbf{z}}} = -y \cdot \frac{(\|\mathbf{z}\|_2\|\hat{\mathbf{z}}\|_2)\mathbf{z} - (\mathbf{z}^T\hat{\mathbf{z}})(\frac{\|\mathbf{z}\|_2}{\|\hat{\mathbf{z}}\|_2})\hat{\mathbf{z}}}{\|\mathbf{z}\|_2^2\|\hat{\mathbf{z}}\|_2^2}$$

ii. (5 points) Compute $\nabla_{\mathbf{W}_2}\mathcal{L}$. For all the following parts, you can use $\delta_{\mathbf{W}_2}$ to refer to $\nabla_{\mathbf{W}_2}\mathcal{L}$.

Solution: Since there are two paths to $\mathbf{W}_2$, so by law of total derivatives

$$\nabla_{\mathbf{W}_2}\mathcal{L} = \frac{\partial \mathbf{z}}{\partial \mathbf{W}_2}\frac{\partial \mathcal{L}}{\partial \mathbf{z}} + \frac{\partial \hat{\mathbf{z}}}{\partial \mathbf{W}_2}\frac{\partial \mathcal{L}}{\partial \hat{\mathbf{z}}}.$$

By the tensor trick learned in class (outer product of two vectors), we have

$$\delta_{\mathbf{W}_2} = \delta_z \mathbf{h}_1^T + \delta_{\hat{\mathbf{z}}} \hat{\mathbf{h}}_1^T$$

iii. (5 points) Compute $\nabla_{\mathbf{h}_1}\mathcal{L}$ and $\nabla_{\hat{\mathbf{h}}_1}\mathcal{L}$. For all the following parts, you can use $\delta_{\mathbf{h}_1}$ and $\delta_{\hat{\mathbf{h}}_1}$ to refer to $\nabla_{\mathbf{h}_1}\mathcal{L}$ and $\nabla_{\hat{\mathbf{h}}_1}\mathcal{L}$ respectively.

Solution: By chain rule,

$$\nabla_{\mathbf{h}_1}\mathcal{L} = \frac{\partial \mathbf{z}}{\partial \mathbf{h}_1}\frac{\partial \mathcal{L}}{\partial \mathbf{z}}$$

$$\nabla_{\hat{\mathbf{h}}_1}\mathcal{L} = \frac{\partial \hat{\mathbf{z}}}{\partial \hat{\mathbf{h}}_1}\frac{\partial \mathcal{L}}{\partial \hat{\mathbf{z}}}.$$

Since,

$$\frac{\partial \mathbf{z}}{\partial \mathbf{h}_1} = \frac{\partial \hat{\mathbf{z}}}{\partial \hat{\mathbf{h}}_1} = \mathbf{W}_2^T,$$

so

$$\delta_{\mathbf{h}_1} = \mathbf{W}_2^T \delta_{\mathbf{z}}$$

$$\delta_{\hat{\mathbf{h}}_1} = \mathbf{W}_2^T \delta_{\hat{\mathbf{z}}}.$$

iv. (5 points) Compute $\nabla_{\mathbf{m}}\mathcal{L}$ and $\nabla_{\mathbf{n}}\mathcal{L}$. For all the following parts, you can use $\delta_{\mathbf{m}}$ and $\delta_{\mathbf{n}}$ to refer to $\nabla_{\mathbf{m}}\mathcal{L}$ and $\nabla_{\mathbf{n}}\mathcal{L}$ respectively. Use the symbol $\odot$ to denote elementwise multiplication (Hadamard product).

Solution: By chain rule,

$$\nabla_{\mathbf{m}}\mathcal{L} = \frac{\partial \mathbf{h}_1}{\partial \mathbf{m}}\frac{\partial \mathcal{L}}{\partial \mathbf{h}_1}$$

$$\nabla_{\mathbf{n}}\mathcal{L} = \frac{\partial \hat{\mathbf{h}}_1}{\partial \mathbf{n}}\frac{\partial \mathcal{L}}{\partial \hat{\mathbf{h}}_1}.$$

Since ReLU gate routes the gradient, so

$$\delta_{\mathbf{m}} = \mathbb{1}(\mathbf{m} \geq 0) \odot \delta_{\mathbf{h}_1}$$

$$\delta_{\mathbf{n}} = \mathbb{1}(\mathbf{n} \geq 0) \odot \delta_{\hat{\mathbf{h}}_1}$$

v. (5 points) Compute $\nabla_{\mathbf{W}_1}\mathcal{L}$.

Solution: Since there are two paths to $\mathbf{W}_1$, so by law of total derivatives

$$\nabla_{\mathbf{W}_1}\mathcal{L} = \frac{\partial \mathbf{m}}{\partial \mathbf{W}_1}\frac{\partial \mathcal{L}}{\partial \mathbf{m}} + \frac{\partial \mathbf{n}}{\partial \mathbf{W}_1}\frac{\partial \mathcal{L}}{\partial \mathbf{n}}.$$

By the tensor trick learned in class (outer product of two vectors), we have

$$\delta_{\mathbf{W}_1} = \delta_{\mathbf{m}}\mathbf{x}^T + \delta_{\mathbf{n}}\hat{\mathbf{x}}^T$$

(b) (9 points) In the similarity network architecture, $\mathbf{z}$ and $\hat{\mathbf{z}}$ represents the embedding vectors for input signature images $\mathbf{x}$ and $\hat{\mathbf{x}}$ respectively. Suppose we are given a training sample, $\{(\mathbf{x}^{(g)}, \hat{\mathbf{x}}^{(g)}), +1\}$.

i. (3 points) Compute the loss for the training sample if $\mathbf{z}^{(g)} = \hat{\mathbf{z}}^{(g)}$.

Solution: If $\mathbf{z}^{(g)} = \hat{\mathbf{z}}^{(g)}$, then

$$s^{(g)} = \cos\langle \mathbf{z}^{(g)}, \hat{\mathbf{z}}^{(g)}\rangle$$
$$= 1.$$

Therefore,

$$\mathcal{L}^{(g)} = -1 \cdot s^{(g)}$$
$$= -1.$$

ii. (3 points) Compute the loss for the training sample if $\mathbf{z}^{(g)}$ and $\hat{\mathbf{z}}^{(g)}$ are orthogonal to each other

Solution: If $\mathbf{z}^{(g)}$ and $\hat{\mathbf{z}}^{(g)}$ are orthogonal to each other, then

$$s^{(g)} = \cos\langle \mathbf{z}^{(g)}, \hat{\mathbf{z}}^{(g)}\rangle$$
$$= 0.$$

Therefore,

$$\mathcal{L}^{(g)} = -1 \cdot s^{(g)}$$
$$= 0.$$

iii. (3 points) Compute the loss for the training sample if $\mathbf{z}^{(g)} = -\hat{\mathbf{z}}^{(g)}$.

Solution: If $\mathbf{z}^{(g)} = -\hat{\mathbf{z}}^{(g)}$, then

$$s^{(g)} = \cos\langle \mathbf{z}^{(g)}, \hat{\mathbf{z}}^{(g)}\rangle$$
$$= -1.$$

Therefore,

$$\mathcal{L}^{(g)} = -1 \cdot s^{(g)}$$
$$= 1.$$

(c) (1 points) Based on your answer to part (b), explain if the loss function is forcing the embedding vectors in the right direction.

Solution: From part (b), we can see that by minimizing the loss function the embedding vectors for the input pair of images that are genuine are getting forced to be similar to each other (loss for b(i) is the least) which is what we want to achieve for the signature forgery detection application.

3. **Training neural networks** (25 points)

   (a) (4 points) Which of the following activation functions where vanishing gradients usually happen? **Select all that apply.** (Note: Justification is not necessary, but may result in partial credit if the answer is incorrect.)
   A. ReLU
   B. Tanh
   C. Sigmoid
   D. Leaky ReLU
   E. Identity

   Solution: A, B, C.
   A. ReLU saturates for negative values, giving zero gradient.
   B. Like the sigmoid unit, when a unit saturates, i.e., its values grow larger or smaller, the unit saturates and no additional learning occurs.
   C. At extremes, the unit saturates and thus has zero gradient. This results in no learning with gradient descent.

   (b) (5 points) What is **true** about batch normalization? **Select all that apply.** (Note: Justification is not necessary, but may result in partial credit if the answer is incorrect.)
   A. Batch normalization slows down the training process by requiring more iterations.
   B. Batch normalization is a non-learnable transformation.
   C. Batch normalization is a non-linear transformation to make the output of each layer have unit statistics.
   D. Batch normalization introduces noise to a hidden layer's activation.
   E. Batch normalization is not applicable at test time.

   Solution: D.
   A. Batch normalization *accelerates* training by requiring fewer iterations to converge to a given loss value.
   B. Batch normalization has *learnable* parameters
   C. Batch normalization is a linear transformation
   D. It introduces noise to a hidden layer's activation because the mean and the standard deviatio nare *estimated* with a mini-batch of data.
   E. Use the running mean and variance from training statistics instead.

(c) (5 points) Which of the following are **true** about regularization? **Select all that apply.** (Note: Justification is not necessary, but may result in partial credit if the answer is incorrect.)

A. L1 regularization often results in some weights being 0.

B. Adding a regularization penalty will always reduce the training loss.

C. Dropout acts as regularization.

D. Unsuccessful regularization attempts (such as having too large a weight on a parameter norm penalty) could lead to model underfitting.

E. None of the above

Solution: A, C, D.

(d) (5 points) Which of the following are **true**? **Select all that apply.** (Note: Justification is not necessary, but may result in partial credit if the answer is incorrect.)

A. In transfer learning, we can freeze most parameters of the original network

B. Data augmentation could help address the class imbalance problem for image classification

C. Multitask learning is not applicable if you have a small amount of data for a particular task

D. Ensemble methods are an effective way to improve performance

E. None of the above

Solution: A, B, D.

(e) (6 points) Early stopping is a popular regularization method that constantly evaluates the training and validation loss on each training iteration, and returns the model with the lowest validation error. Now, you are going to draw an illustration of early stopping and introduce the concept of it to your friend. Fill in the blanks in the figure with precise answers.
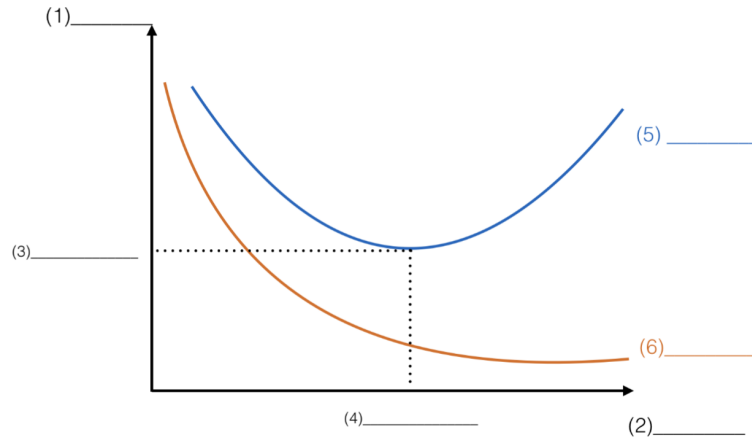
Hint:
(1) and (2) describe the axis legends.
(3) and (4) describe specific values on the vertical and horizontal axes.
(5) and (6) describe the names of curves.

Solution:
(1) Loss (or error)
(2) Number of iterations (or number of epochs)
(3) Best validation loss value (or best validation error)
(4) Optimal stopping point (or early stopping point)
(5) Validation loss (or validation error)
(6) Training loss (or training error)

4. **Gradient-based optimization algorithms** (15 points)

We have learned several optimization algorithms. Given a loss function $\mathcal{L}(\theta)$, the algorithms make use of the gradient information $\mathbf{g} = \nabla_\theta \mathcal{L}$ to iteratively update the parameters θ. The update rule, however, varies for different algorithms.

Let $\mathbf{g}_t := \nabla_\theta \mathcal{L}(\theta_{t-1})$ be the gradient at θ_{t-1}. This question will discuss the following update rules from class, reproduced here for convenience:

Gradient Descent At the tth iteration,

$$\theta_t \leftarrow \theta_{t-1} - \varepsilon \mathbf{g}_t,$$

where ε is the step size hyperparameter.

Gradient Descent with Momentum At the tth iteration,

$$\mathbf{v}_t \leftarrow \alpha \mathbf{v}_{t-1} - \varepsilon \mathbf{g}_t$$
$$\theta_t \leftarrow \theta_{t-1} + \mathbf{v}_t$$

where ε is the step size hyperparameter, and $\alpha \in [0, 1]$ is the running average parameter for momentum.

AdaGrad At the tth iteration,

$$\mathbf{a}_t \leftarrow \mathbf{a}_{t-1} + \mathbf{g}_t \odot \mathbf{g}_t$$
$$\theta_t \leftarrow \theta_{t-1} - \frac{\varepsilon}{\sqrt{\mathbf{a}_t} + \nu} \odot \mathbf{g}_t,$$

where ν is a small value to prevent zero-division and ε is the step size hyperparameter.

Adam At the tth iteration,

$$\mathbf{v}_t \leftarrow \beta_1 \mathbf{v}_{t-1} + (1 - \beta_1)\mathbf{g}_t$$
$$\mathbf{a}_t \leftarrow \beta_2 \mathbf{a}_{t-1} + (1 - \beta_2)\mathbf{g}_t \odot \mathbf{g}_t$$
$$\tilde{\mathbf{v}}_t = \frac{1}{1 - \beta_1^t} \mathbf{v}_t \qquad \text{(bias correction for first moment)}$$
$$\tilde{\mathbf{a}}_t = \frac{1}{1 - \beta_2^t} \mathbf{a}_t \qquad \text{(bias correction for second moment)}$$
$$\theta_t \leftarrow \theta_{t-1} - \frac{\varepsilon}{\sqrt{\tilde{\mathbf{a}}_t} + \nu} \odot \tilde{\mathbf{v}}_t,$$

where ν is a small value to prevent zero-division, β_1 and β_2 are the running average parameter for the first and second moment estimation. ε is the step size hyperparameter.

(a) (10 points) **Getting out of a "trap"**. Figure 2 is the landscape of a loss function with an 1-D parameter $\theta \in \mathbb{R}$. As the plot shows, there is a "plateau" between $\theta = 3$ and $\theta = 6$.

In the plot, the arrows show 6 vanilla gradient descent steps (with a fixed step size ε) before reaching the red dot near a local minimum. Note that the 6th step is so small that

the details can only be shown in the zoom-in inset. This demonstrates that the plateau acts as a "trap" for gradient descent, where the gradient almost vanishes, leading to marginal update magnitude.

Now consider the optimization algorithms mentioned above. Assume they all share the same ε and starting point as that are used for the plotted gradient descent steps, and that *Adam* and *AdaGrad* share the same ν.

   i. (5 points) Which optimization algorithms would have a better chance to get out of the trap compared to *Gradient Descent*? Briefly explain your reasons.

      Solution: The *Gradient Descent with Momentum* and *Adam* would have better chance to get out of the plateau "trap", because they would be able to gather momentum starting uphill on the left, and even though the gradient vanishes in the plateau, the accumulated momentum will drive the optimizer rightward out of the plateau.

  ii. (5 points) After several updates from the same starting point, when the optimizers "just step into the plateau", please order the "update magnitude" given by *Gradient Descent with Momentum*, *AdaGrad*, and *Adam*. Briefly explain your reasons.

      Here "update magnitude" refers to the norm of the update step, for example, at the tth step, "update magnitude" is $\|\theta_t - \theta_{t-1}\|_2$.

      Solution: The update magnitude order is

>   *Gradient Descent with Momentum* > *Adam* > *AdaGrad*

      Momentum will help increase the update magnitude at the plateau, while *AdaGrad* will shrink the update magnitude. Combining both, *Adam* will give an update magnitude in the middle of the two extremes.
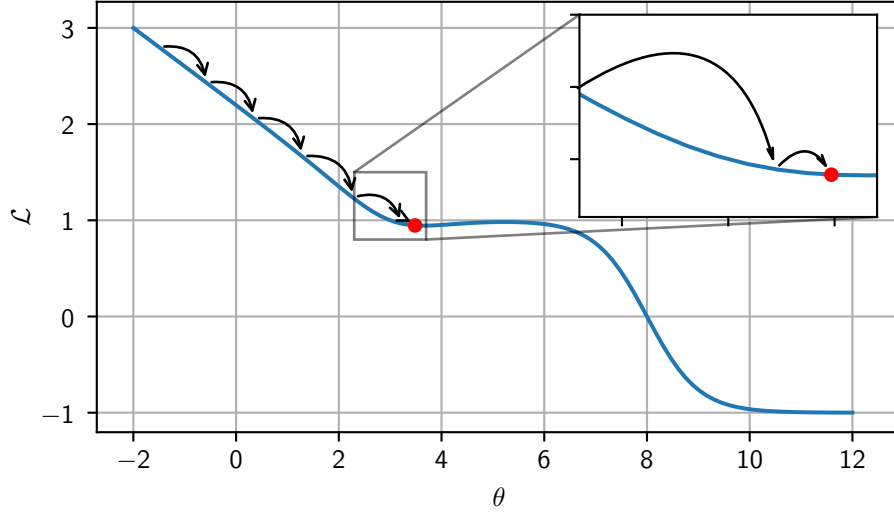
Figure 2: Loss landscape of $\mathcal{L}(\theta)$, and a gradient descent trajectory on it.

(b) (5 points) Notice that the Adam algorithm designs the "bias correction" steps for the first and second moment estimation of the gradients. In this question, we are going to derive the correction factors.

We will treat the gradients along the optimization trajectory as random variables, and assume that $\mathbf{g}_1, \mathbf{g}_2, \ldots$, are i.i.d. with some distribution that has the first and second moment. That is, we assume

$$\mathbb{E}[\mathbf{g}_t] = \boldsymbol{\mu}, \quad t = 1, 2, \ldots$$
$$\mathbb{E}[\mathbf{g}_t^2] = \mathbf{s}, \quad t = 1, 2, \ldots$$

where for simplicity, we denote $\mathbf{g}_t \odot \mathbf{g}_t$ as $\mathbf{g}_t^2$.

We first expand the recursive relation and express $\mathbf{v}_t$ in terms of $\mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_t$. This gives

$$\mathbf{v}_t = (1 - \beta_1)\mathbf{g}_t + \beta_1(1 - \beta_1)\mathbf{g}_{t-1} + \beta_1^2(1 - \beta_1)\mathbf{g}_{t-2} + \ldots + \beta_1^{t-1}(1 - \beta_1)\mathbf{g}_1$$

$$= (1 - \beta_1)\sum_{i=1}^{t} \beta_1^{t-i}\mathbf{g}_i \tag{1}$$

and similarly,

$$\mathbf{a}_t = (1 - \beta_2)\sum_{i=1}^{t} \beta_2^{t-i}\mathbf{g}_i^2 \tag{2}$$

Then consider the expectation of $\mathbf{v}_t$, $\mathbb{E}[\mathbf{v}_t]$, and compare with $\boldsymbol{\mu}$.

15

Show that the correction factor $\gamma_1 = \dfrac{1}{1 - \beta_1^t}$ satisfies

$$\gamma_1 \mathbb{E}[\mathbf{v}_t] = \boldsymbol{\mu} = \mathbb{E}[\mathbf{g}_t].$$

You will see that $\gamma_2 = \dfrac{1}{1 - \beta_2^t}$ corrects $\mathbb{E}[\mathbf{a}_t]$ to $\mathbf{s}$ (i.e. $\mathbb{E}[\mathbf{g}_t^2]$) in a similar way.

Hint: The sum of a geometric series $p^0, p^1, \ldots, p^{n-1}$ is given by:

$$\sum_{j=1}^{n-1} p^j = \frac{1 - p^n}{1 - p}$$

Solution: Change the time index variable i to $j = t - i$, then $\mathbf{v}_t = (1 - \beta_1) \displaystyle\sum_{j=0}^{t-1} \beta_1^j \mathbf{g}_{t-j}$.

Now

$$\mathbb{E}[\mathbf{v}_t] = (1 - \beta_1) \sum_{j=0}^{t-1} \beta_1^j \, \mathbb{E}[\mathbf{g}_{t-j}] = (1 - \beta_1) \frac{1 - \beta_1^t}{1 - \beta_1} \boldsymbol{\mu} = (1 - \beta_1^t) \boldsymbol{\mu} = \frac{1}{\gamma_1} \boldsymbol{\mu}$$

Similarly,

$$\mathbb{E}[\mathbf{a}_t] = (1 - \beta_2) \sum_{j=0}^{t-1} \beta_2^j \, \mathbb{E}[\mathbf{g}_{t-j}^2] = (1 - \beta_2) \frac{1 - \beta_2^t}{1 - \beta_2} \mathbf{s} = (1 - \beta_2^t) \mathbf{s} = \frac{1}{\gamma_2} \mathbf{s}$$

5. **Bonus** (5 points) **Nesterov Momentum**.

Recall that in class, we discussed the Nesterov momentum update. For parameters θ, Nesterov momentum performs:

$$\begin{aligned} \mathbf{v} &\leftarrow \alpha\mathbf{v} - \epsilon\nabla_\theta\mathcal{L}(\theta + \alpha\mathbf{v}) \\ \theta &\leftarrow \theta + \mathbf{v} \end{aligned}$$

In class, we showed the result that by defining $\tilde{\theta}_{\text{old}} = \theta_{\text{old}} + \alpha\mathbf{v}_{\text{old}}$, the update becomes:

$$\begin{aligned} \mathbf{v}_{\text{new}} &= \alpha\mathbf{v}_{\text{old}} - \epsilon\nabla_\theta\mathcal{L}(\tilde{\theta}_{\text{old}}) \\ \tilde{\theta}_{\text{new}} &= \tilde{\theta}_{\text{old}} + \mathbf{v}_{\text{new}} + \alpha(\mathbf{v}_{\text{new}} - \mathbf{v}_{\text{old}}) \end{aligned}$$

followed by setting $\mathbf{v}_{\text{old}} = \mathbf{v}_{\text{new}}$ and $\tilde{\theta}_{\text{old}} = \tilde{\theta}_{\text{new}}$. Show that these two update rules are equivalent.

Solution: The first equation,

$$\mathbf{v}_{\text{new}} = \alpha\mathbf{v}_{\text{old}} - \epsilon\nabla_\theta\mathcal{L}(\tilde{\theta}_{\text{old}})$$

follows from substituting the definition of $\tilde{\theta}$ into $\mathbf{v} \leftarrow \alpha\mathbf{v} - \epsilon\nabla_\theta\mathcal{L}(\theta + \alpha\mathbf{v})$. For the second equation, note:

$$\begin{aligned} \tilde{\theta}_{\text{new}} &= \theta_{\text{new}} + \alpha\mathbf{v}_{\text{new}} \\ &= \theta_{\text{old}} + \mathbf{v}_{\text{new}} + \alpha\mathbf{v}_{\text{new}} \\ &= \tilde{\theta}_{\text{old}} - \alpha\mathbf{v}_{\text{old}} + \mathbf{v}_{\text{new}} + \alpha\mathbf{v}_{\text{new}} \\ &= \tilde{\theta}_{\text{old}} + \mathbf{v}_{\text{new}} + \alpha(\mathbf{v}_{\text{new}} - \mathbf{v}_{\text{old}}) \end{aligned}$$

where in the second line, we used $\theta_{\text{new}} = \theta_{\text{old}} + \mathbf{v}_{\text{new}}$ and the third line, we used $\theta_{\text{old}} = \tilde{\theta}_{\text{old}} - \alpha\mathbf{v}_{\text{old}}$.