%matplotlib inline %load ext autoreload %autoreload 2 import matplotlib.pyplot as plt import numpy as np import os import pandas as pd from scipy.special import expit from aml utils import test case checker, perform computation, show test cases 0. Data Since the MNIST data (http://yann.lecun.com/exdb/mnist/) is stored in a binary format, we would rather have an API handle the loading for us. Pytorch (https://pytorch.org/) is an Automatic Differentiation library that we may see and use later in the course. Torchvision (https://pytorch.org/docs/stable/torchvision/index.html?highlight=torchvision#moduletorchvision) is an extension library for pytorch that can load many of the famous data sets painlessly. We already used Torchvision for downloading the MNIST data. It is stored in a numpy array file that we will load easily. 0.1 Loading the Data if os.path.exists('../MeanField-lib/mnist.npz'): npzfile = np.load('../MeanField-lib/mnist.npz') train images raw = npzfile['train_images_raw'] train labels = npzfile['train_labels'] eval images raw = npzfile['eval images raw'] eval labels = npzfile['eval labels'] else: import torchvision download = not os.path.exists('../MeanField-lib/mnist') data train = torchvision.datasets.MNIST('.../MeanField-lib/mnist', train=True, train data eval = torchvision.datasets.MNIST('../MeanField-lib/mnist', train=False, train train_images_raw = data_train.data.numpy() train labels = data train.targets.numpy() eval images raw = data eval.data.numpy() eval_labels = data_eval.targets.numpy() np.savez('../MeanField-lib/mnist.npz', train_images_raw=train_images_raw, train_la eval images raw=eval images raw, eval labels=eval labels) noise flip prob = 0.04Task 1 Write the function get_thresholded_and_noised that does image thresholding and flipping pixels. More specifically, this functions should exactly apply the following two steps in order: 1. Thresholding: First, given the input threshold argument, you must compute a thresholded image array. This array should indicate whether each element of images_raw is greater than or equal to the threshold argument. We will call the result of this step the thresholded image. 2. Noise Application (i.e., Flipping Pixels): After the image was thresholded, you should use the flip_flags input argument and flip the pixels with a corresponding True entry in flip_flags. flip_flags mostly consists of False entries, which means you should not change their corresponding pixels. Instead, whenever a pixel had a True entry in flip_flags , that pixel in the thresholded image must get flipped. This way you will obtain the noised image. 3. Mapping Pixels to -1/+1: You need to make sure the output image pixels are mapped to -1 and 1 values (as opposed to 0/1 or True/False). get_thresholded_and_noised should take the following arguments: 1. images_raw: A numpy array. Do not assume anything about its shape, dtype or range of values. Your function should be careless about these attributes. 2. threshold: A scalar value. 3. flip_flags: A numpy array with the same shape as images_raw and np.bool dtype. This array indicates whether each pixel should be flipped or not. and return the following: mapped_noised_image: A numpy array with the same shape as images_raw. This array's entries should either be -1 or 1. **Notes** numpy.where(condition, x, y): Return elements chosen from x or y depending on condition. Parameters: • condition: array_like, or bool: Where True, yield x, otherwise yield y. x, y: array_like: Values from which to choose. x, y and condition need to be broadcastable to some shape. Returns: • out: ndarray: An array with elements from x where condition is True, and elements from y elsewhere. 1. indicate whether each element of images_raw is greater than or equal to 'threshold' => thresholded image A. Calculate the shed_image array using boolean array check on images_raw. 2. if flip_flags pixel == True that pixel in the thresholded image must get flipped => noised A. Using logical_not function you create a not_threshed_image array which is logical not of threshed_image. B. Use numpy where function to check condition flip_flags == True and return either value from not_threshed_image or threshed_image. 3. Output image pixels in (-1, 1) Use numpy.where and numpy.logical_not How to apply numpy.logical_not using the index produced in the numpy.where: -return a truth array. -1 if your image is less than threshhold, +1 if your image is larger than threshhold 1. get a true/false mask based off the threshhold value. 2. use flip_flags to flip this true/false mask. Flip flags is just a matrix of true/false. just use it to index into the matrix you wish to flip values for. 3. get mapped_noised_image by the logic: if the mask entry is True --> then use values of 1, else use values of -1. 4. comparison between images_raw and threshold and save results. 5. use np.logical_not and np where to find where flip flags is true and return result of my result of np.logical_not. result = np.logical_not(step1) result[np.where(flip_flags == True)]. noised = thresholded flip_flags where, thresholded is the array from step 1 6. convert boolean results to int values. In [4]: def get_thresholded_and_noised(images_raw, threshold, flip_flags): # Beginning of Mo's code #1. indicate whether each element of images raw is greater than or equal to 'thre #1. Calculate theshed image array using boolean array check on images raw. thresholded = images raw >= threshold #2 np.logical not(x, out, where) noised = thresholded np.logical not(thresholded, out=noised, where=flip flags.astype(bool)) #3 mapped noised image = np.where(noised == True, 1, -1) # End of Mo's code assert (np.abs(mapped noised image) == 1).all() return mapped noised image.astype(np.int32) # This cell is left empty as a seperator. You can leave this cell as it is, and you si # Performing sanity checks on your implementation **def** test thresh noise(x, seed = 12345, p = noise flip prob, threshold = 128): np random = np.random.RandomState(seed=seed) flip flags = (np random.uniform(0., 1., size=x.shape) < p)</pre> return get thresholded and noised(x, threshold, flip flags) (orig image, ref image, test im, success thr) = show test cases(test thresh noise, tast assert success thr # Checking against the pre-computed test database test results = test case checker(get thresholded and noised, task id=1) assert test results['passed'], test results['message'] The reference and solution images are the same to a T! Well done on this test case. Reference Solution Image Raw Image Your Solution Image 10 Enter nothing to go to the next image Enter "s" when you are done to recieve the three images. **Don't forget to do this before continuing to the next step.** # This cell is left empty as a seperator. You can leave this cell as it is, and you si 0.2 Applying Thresholding and Noise to Data if perform computation: X_true_grayscale = train_images_raw[:10, :, :] np random = np.random.RandomState(seed=12345) flip_flags = flip_flags = (np_random.uniform(0., 1., size=X_true_grayscale.shape) initial_pi = np_random.uniform(0, 1, size=X_true_grayscale.shape) # Initial Random X true = get thresholded_and_noised(X_true_grayscale, threshold=128, flip_flags=fl X_noised = get_thresholded_and_noised(X_true_grayscale, threshold=128, flip flags= Task 2 Write a function named $sigmoid_2x$ that given a variable X computes the following: $f(X) := rac{\exp(X)}{\exp(X) + \exp(-X)}$ The input argument is a numpy array X, which could have any shape. Your output array must have the same shape as X. **Important Note**: Theoretically, f satisfies the following equations: $\lim_{X o +\infty} f(X) = 1$ $\lim_{X \to -\infty} f(X) = 0$ Your implementation must also work correctly even on these extreme edge cases. In other words, you must satisfy the following tests. sigmoid_2x(np.inf)==1 $sigmoid_2x(-np.inf)==0$. **Hint**: You may find scipy.special.expit useful. divide numerator and denominator of expit $f(X) := \frac{\exp(X)}{\exp(X) + \exp(-X)}$ by $\exp(X)$ to get $\frac{1}{1 + \exp(-2X)}$ In [9]: **def** sigmoid 2x(X): # Beginning of Mo's code output = expit(2*X)# End of Mo's code return output # Performing sanity checks on your implementation assert sigmoid_2x(+np.inf) == 1. **assert** $sigmoid_2x(-np.inf) == 0.$ assert np.array equal(sigmoid 2x(np.array([0, 1])).round(3), np.array([0.5, 0.881])) # Checking against the pre-computed test database test_results = test_case_checker(sigmoid_2x, task_id=2) assert test_results['passed'], test_results['message'] # This cell is left empty as a seperator. You can leave this cell as it is, and you si 1. Applying Mean-field Approximation to Boltzman Machine's Variational Inference Problem Task 3 Write a boltzman_meanfield function that applies the mean-field approximation to the Boltzman machine. Recalling the textbook notation, X_i is the observed value of pixel i, and H_i is the true value of pixel i(before applying noise). For instance, if we have a 3 imes 3 image, the corresponding Boltzman machine looks like this: Here, we a adopt a slightly simplified notation from the textbook and define $\mathcal{N}(i)$ to be the neighbors of pixel i (the pixels adjacent to pixel i). For instance, in the above figure, we have $\mathcal{N}(1)=\{2,4\}$, $\mathcal{N}(2) = \{1, 3, 5\}$, and $\mathcal{N}(5) = \{2, 4, 6, 8\}$. With this, the process in the textbook can be summarized as follows: 1. for iteration = 1, 2, 3,, 2. Pick a random pixel i. 3. Find pixel i's new parameter as $\pi_i^{ ext{new}} = rac{\exp(heta_{ii}^{(2)} X_i + \sum_{j \in \mathcal{N}(i)} heta_{ij}^{(1)} (2\pi_j - 1))}{\exp(heta_{ii}^{(2)} X_i + \sum_{j \in \mathcal{N}(i)} heta_{ij}^{(1)} (2\pi_j - 1)) + \exp(- heta_{ii}^{(2)} X_i - \sum_{j \in \mathcal{N}(i)} heta_{ij}^{(1)} (2\pi_j - 1))}.$ 4. Replace the existing parameter for pixel i with the new one. $\pi_i \leftarrow \pi_i^{\text{new}}$ Since our computational resources are extremely vectorized, we will make the following minor algorithmic modification and ask you to implement the following instead: 1. for iteration = 1, 2, 3,, 2. for each pixels i: 3. Find pixel i's new parameter, but do not update the original parameter yet. $\pi_i^{ ext{new}} = rac{\exp(heta_{ii}^{(2)} X_i + \sum_{j \in \mathcal{N}(i)} heta_{ij}^{(1)} (2\pi_j - 1))}{\exp(heta_{ii}^{(2)} X_i + \sum_{j \in \mathcal{N}(i)} heta_{ij}^{(1)} (2\pi_j - 1)) + \exp(- heta_{ii}^{(2)} X_i - \sum_{j \in \mathcal{N}(i)} heta_{ij}^{(1)} (2\pi_j - 1))}.$ 4. Once you have computed all the new parameters, update all of them at the same time: $\pi \leftarrow \pi^{\text{new}}$ We assume that the parameters $heta_{ii}^{(2)}$ have the same value for all i and denote their common value by scalar <code>theta_X</code> . Moreover, we assume that the parameters $heta_{ij}^{(1)}$ have the same value for all i,j and denote their common value by scalar theta_pi. The boltzman_meanfield function must take the following input arguments: 1. images: A numpy array with the shape (N,height,width), where N is the number of samples and could be anything, height is each individual image's height in pixels (i.e., number of rows in each image), • and width is each individual image's width in pixels (i.e., number of columns in each image). Do not assume anything about images 's dtype or the number of samples or the height ■ The entries of images are either -1 or 1. 2. initial_pi : A numpy array with the same shape as images (i.e. (N,height,width)). This variable is corresponding to the initial value of π in the textbook analysis and above equations. Note that for each of the N images, we have a different π variable. 3. theta_X: A scalar with a default value of 0.5*np.log(1/noise_flip_prob-1). This variable represents $\theta_{ii}^{(2)}$ in the above update equation. 4. theta_pi : A scalar with a default value of 2. This variable represents $\theta_{ij}^{(1)}$ in the above update equation. 5. iterations: A scalar with a default value of 100. This variable denotes the number of update iterations to perform. The boltzman_meanfield function must return the final π variable as a numpy array called pi , and should contain values that are between 0 and 1. **Hint**: You may find the sigmoid_2x function, that you implemented earlier, useful. Hint: If you want to find the summation of neighboring elements for all of a 2-dimensional matrix, there is an easy and efficient way using matrix operations. You can initialize a zero matrix, and then add four shifted versions (i.e., left-, right-, up-, and down-shifted versions) of the original matrix to it. You will have to be careful in the assignment and selection indices, since you will have to drop one row/column for each shifted version of the matrix. **Important Note**: Do **not** use np.roll if you're taking this approach. **Important Note**: When evaluating the neighborhood sum experssions (i.e., terms with $\sum_{i \in \mathcal{N}(i)}$), make sure that you do not inadvertently include a "ghost" pixel in $\mathcal{N}(i)$. For instance, make sure you're only using H_5, H_7, H_9, and X_8 when computing an update for H_8. That is, only left-, right-, and down-shifted pixels should be contributing to H_8 's neighourhood sums. If you mistakenly add an upshifted pixel to H_8 's neighourhood sums (whether it's a copy of H_8 or a no-ink/zero pixel), you are effectively imposing an extra neighborhood edge between H_8 and a "ghost" pixel below it; notice that our boltzman machine doesn't have a neighborhood edge between H_8 and anything below it, therefore, neither H_8 nor an extra non-inky pixel should be participating in H_8 's neighborhood sums and update. Missing this point can cause an initial mismatche in the edge pixel updates, which will be disseminated through iterative updates to other pixels. **Notes** 1. Create a separate function which uses matrix operations to calculate sum of neighboring elements of 2. For each iteration: For each pi get neighboring value sum array using step 1 function lacksquare Calculate the term for updating parameters: $heta_{ii}^{(2)}X_i+\sum_{j\in\mathcal{N}(i)} heta_{ij}^{(1)}\left(2\pi_j-1
ight)$ 1. Pass above term through sigmoid_2x function to get updated value for π def boltzman meanfield(images, initial pi, theta X=0.5*np.log(1/noise flip prob-1), the X=0.5*np. if len(images.shape) === 2: # In case a 2d image was given as input, we'll add a dummy dimension to be con X = images.reshape(1,*images.shape) # Otherwise, we'll just work with what's given X = imagespi = initial pi # Beginning of Mo's code #1 Create a separate function which uses matrix operations to calculate sum of ne def shift(pi, right, up): e = np.empty like(pi) **if** right >= 0: e[:, :right, :] = 0e[:, right:, :] = pi[:, :-right, :] e[:, right:, :] = 0e[:, :right, :] = pi[:, -right:, :] **if** up >= 0: e[:, :, :up] = 0e[:, :, up:] = pi[:, :, :-up] e[:, :, up:] = 0e[:, :, :up] = pi[:, :, -up:] def SumNi(pi): #Ni = shift(pi, 1, 0) + shift(pi, -1, 0) + shift(pi, 0, 1) + shift(pi, 0, -1)#left[left!=0]=2*left[left!=0]-1 ##from campuswire??? #do I multiply all pi here by theta pi? r = shift(pi, 1, 0)[shift(pi, 1, 0) !=0] = 2 * shift(pi, 1, 0)[shift(pi, 1, 0)]1 = shift(pi, -1, 0) [shift(pi, -1, 0) !=0] = 2 * shift(pi, -1, 0) [shift(pi, -1, 0) !=0]d = shift(pi, 0, -1)[shift(pi, 0, -1) !=0] = 2 * shift(pi, 0, -1)[shift(pi, 0, -1)]u = shift(pi, 0, 1)[shift(pi, 0, 1) !=0] = 2 * shift(pi, 0, 1)[shift(pi, 0, 0, 1)]Ni = r + l + d + ureturn Ni #do I replace pi with theta pi * (2 * pi - 1) for i in range(iterations): #2 - get neighboring value sum array using step 1 function # - Calculate the term for updating parameters $\#cmn \ term = theta \ X * X + SumNi(pi) * theta pi * (2 * pi - 1)$ cmn term = theta X * X + SumNi(theta pi * (2 * pi - 1))#3 Pass above term through sigmoid 2x function to get updated value for pi pi = sigmoid 2x(cmn term) # End of Mo's code return pi.reshape(*images.shape) # This cell is left empty as a seperator. You can leave this cell as it is, and you si In [14]: # Performing sanity checks on your implementation def test boltzman(x, seed = 12345, theta X=0.5*np.log(1/noise flip prob-1), theta pi=2 np_random = np.random.RandomState(seed=seed) initial pi = np random.uniform(0,1, size=x.shape) return boltzman_meanfield(x, initial_pi, theta_X=theta_X, theta pi=theta pi, iterations=iterations) (orig_image, ref_image, test_im, success_is_row_inky) = show_test_cases(test_boltzman) assert success_is_row_inky # Checking against the pre-computed test database test results = test case checker(boltzman meanfield, task id=3) assert test results['passed'], test results['message'] Traceback (most recent call last) ValueError Input In [14], in <module> initial_pi = np_random.uniform(0,1, size=x.shape) return boltzman meanfield(x, initial pi, theta X=theta X, theta_pi=theta_pi, iterations=iterations) ----> 8 (orig_image, ref_image, test_im, success_is_row_inky) = <mark>show_test_cases(test_b</mark> oltzman, task_id='3_V') 10 assert success is row inky 12 # Checking against the pre-computed test database File ~/work/release/MeanField-lib/aml_utils.py:451, in show_test_cases(test_func, task 449 orig images = npz file['raw images'] 450 ref_images = npz_file['ref_images'] --> 451 test_images = test_func(orig_images) **453** rtol = 1e-05 454 if ('meanfield' in this_dir.lower()) and ('3' in str(task_id)): Input In [14], in test boltzman(x, seed, theta X, theta pi, iterations) 3 np random = np.random.RandomState(seed=seed) 4 initial pi = np random.uniform(0,1, size=x.shape) ----> 5 return boltzman_meanfield(x, initial_pi, theta_X=theta_X, theta_pi=theta_pi, iterations=iterations) Input In [12], in boltzman meanfield(images, initial pi, theta X, theta pi, iteration 43 #do I replace pi with theta_pi * (2 * pi - 1) **44 for** i **in** range(iterations): #2 - get neighboring value sum array using step 1 function
- Calculate the term for updating parameters 45 46 #cmn_term = theta_X * X + SumNi(pi) * theta_pi * (2 * pi - 1)
cmn_term = theta_X * X + SumNi(theta_pi * (2 * pi - 1)) 47 --> 49 51 #3 Pass above term through sigmoid_2x function to get updated value for pi pi = sigmoid_2x(cmn_term) Input In [12], in boltzman meanfield.<locals>.SumNi(pi) 32 def SumNi(pi): 33 #Ni = shift(pi, 1, 0) + shift(pi, -1, 0) + shift(pi, 0, 1) + shift(pi, 0, -1) #original #left[left!=0]=2*left[left!=0]-1 ##from campuswire??? #do I multiply all pi here by theta pi? 35 r = shift(pi, 1, 0) [shift(pi, 1, 0) !=0] = 2 * shift(pi, 1, 0) [shift(pi, 1, 0)]**--->** 36 1, 0) != 0] - 1 -1, 0) != 0] -138 d = shift(pi, 0, -1)[shift(pi, 0, -1) !=0] = 2 * shift(pi, 0, -1)[shift(pi, 0, -1)]i, 0, -1) != 0] - 1Input In [12], in boltzman_meanfield.<locals>.shift(pi, right, up) **22** if up >= 0: e[:, :, :up] = 0 e[:, :, up:] = pi[:, :, :-up] 25 else: e[:, :, up:] = 0ValueError: could not broadcast input array from shape (100,28,0) into shape (100,28,2 8) # This cell is left empty as a seperator. You can leave this cell as it is, and you si 2. Tuning the Boltzman Machine's Hyper-Parameters Now, with the boltzman_meanfield function that you implemented above, here see the effect of changing hyper parameters theta_X and theta_pi which were defined in Task 3. We set theta_X to be 0.5*np.log(1/noise_flip_prob-1) where noise_flip_prob was the probability of flipping each pixel. Try to think why this is a reasonable choice. (This is also related to one of the questions in the follow-up quiz). • We try different values for theta_pi. For each value of theta_pi, we the apply the denoising and compare the denoised images to the original ones. We adopt several statistical measures to compare original and denoised images and to finally decide which value of theta_pi is better. Remember that during the noising process, we chose some pixels and decide to flip them, and during the denoising process we essentially try to detect such pixels. Let P be the total number of pixels that we flip during the noise adding process, and N be the total number of pixels that we do not flip during the noise adding process. We can define: True Positive (TP). Defined to be the total number of pixels that are flipped during the noise adding process, and we successfully detect them during the denoising process. True Positive Rate (TPR). Other names: sensitivity, recall. Defined to be the ratio TP / P. False Positive (FP). Defined to be the number of pixels that were detected as being noisy during the denosing process, but were not really noisy. • False Positive Rate (FPR). Other name: fall-out. Defined to be the ratio FP/N. Positive Predictive Value (PPV). Other name: precision. Defined to be the ratio TP / (TP + FP). F1 score. Defined to be the harmonic mean of precision (PPV) and recall (TPR), or equivalently 2 TP / (2 TP + FP + FN). Since we fix theta_X in this section and evaluate different values of theta_pi , in the plots, theta refers to theta_pi. def get_tpr(preds, true_labels): TP = (preds * (preds == true labels)).sum() P = true labels.sum() **if** P==0: TPR = 1.else: TPR = TP / Preturn TPR def get_fpr(preds, true_labels): FP = (preds * (preds != true labels)).sum() N = (1-true labels).sum()**if** N==0: FPR=1 FPR = FP / N return FPR def get_ppv(preds, true_labels): TP = (preds * (preds == true labels)).sum() FP = (preds * (preds != true labels)).sum() **if** (TP + FP) == 0: PPV = 1PPV = TP / (TP + FP)return PPV def get_f1(preds, true_labels): TP = (preds * (preds == true_labels)).sum() FP = (preds * (preds != true_labels)).sum() FN = ((1-preds) * (preds != true labels)).sum() if (2 * TP + FP + FN) == 0: F1 = 1F1 = (2 * TP) / (2 * TP + FP + FN)return F1 if perform computation: $all_theta = np.arange(0, 10, 0.2).tolist() + np.arange(10, 100, 5).tolist()$ tpr list, fpr list, ppv list, f1 list = [], [], [] for theta in all_theta: meanfield_pi = boltzman_meanfield(X_noised, initial_pi, theta_X=0.5*np.log(1/r $X_{denoised} = 2 * (meanfield_pi > 0.5) - 1$ predicted_noise_pixels = (X_denoised != X_noised) tpr = get tpr(predicted noise pixels, flip flags) fpr = get_fpr(predicted_noise_pixels, flip_flags) ppv = get ppv(predicted noise pixels, flip flags) f1 = get_f1(predicted_noise_pixels, flip_flags) tpr_list.append(tpr) fpr_list.append(fpr) ppv_list.append(ppv) f1_list.append(f1) In []: if perform_computation: fig, axes = plt.subplots(nrows=1, ncols=2, figsize=(12,4), dpi=90) ax=axes[0] ax.plot(all_theta, tpr_list) ax.set_xlabel('Theta') ax.set_ylabel('True Positive Rate') ax.set_title('True Positive Rate Vs. Theta') ax.set xscale('log') ax=axes[1] ax.plot(all_theta, fpr_list) ax.set_xlabel('Theta') ax.set_ylabel('False Positive Rate') ax.set_title('False Positive Rate Vs. Theta') ax.set xscale('log') if perform_computation: fig, axes = plt.subplots(nrows=1, ncols=3, figsize=(12,3), dpi=90) ax=axes[0]ax.plot(fpr list, tpr list) ax.set_xlabel('False Positive Rate') ax.set_ylabel('True Positive Rate') ax.set_title('ROC Curve') ax.set xlim(-0.05, 1.05) $ax.set_ylim(-0.05, 1.05)$ ax.plot(np.arange(-0.05, 1.05, 0.01), np.arange(-0.05, 1.05, 0.01), ls='--', c='bl ax=axes[1]ax.plot(all_theta, f1_list) ax.set_xlabel('Theta') ax.set_ylabel('F1-statistic') ax.set_title('F1-score Vs. Theta') ax.set_xscale('log') ax=axes[2] ax.plot(tpr_list, ppv_list) ax.set_xlabel('Recall') ax.set_ylabel('Precision') ax.set title('Precision Vs. Recall') $ax.set_xlim(-0.05, 1.05)$ $ax.set_ylim(-0.05, 1.05)$ ax.plot(np.arange(-0.05, 1.05, 0.01), 1-np.arange(-0.05, 1.05, 0.01), 1s='--', c='--'if perform computation: best_theta = all_theta[np.argmax(f1_list)] print(f'Best theta w.r.t. the F-score is {best_theta}') Now let's try the tuned hyper-parameters, and verify whether it visually improved the Boltzman machine. # This cell is left empty as a seperator. You can leave this cell as it is, and you si if perform_computation: def test_boltzman(x, seed = 12345, theta_X=0.5*np.log(1/noise_flip_prob-1), theta_ np_random = np.random.RandomState(seed=seed) initial_pi = np_random.uniform(0,1, size=x.shape) return boltzman_meanfield(x, initial_pi, theta_X=theta_X, theta_pi=theta_pi, iterations=iterations) > 0.5 (orig image, ref image, test im, success is row inky) = show test cases(test boltz