In [2]:	Ullrich Köthe: Machine Learning Essentials, Summer Semester 2023 Notebook adapted by Daniel Galperin, Fritz Haltenberger Solutions for Exercise 1 Import libraries import numpy as np
	<pre>import matplotlib.pyplot as plt %matplotlib inline import sklearn from sklearn.datasets import load_digits from sklearn import model_selection from sklearn.model_selection import train_test_split, cross_val_score from sklearn.discriminant_analysis import LinearDiscriminantAnalysis</pre> 1 Exploring the Data
In [3]:	<pre># load digits data set digits = load_digits() data</pre>
	<pre>axes[0].imshow(img, cmap="gray", interpolation="nearest") axes[0].set_axis_off() axes[1].imshow(img, cmap="gray", interpolation="bilinear") axes[1].set_axis_off() axes[2].imshow(img, cmap="gray", interpolation="bicubic") axes[2].set_axis_off() plt.show() data.shape</pre>
	<pre>images.shape</pre>
In [4]:	The right-most image illustrates why we generally use interpolation = 'nearest'. For scientific analysis, it's important that we can see the exact value of each pixel in an image array, even if interpolation = 'bicubic' often yields visually more pleasing results. If your image has the shape (width, height) matplotlib will display it using a colormap, viridis by default. You can change the cmap parameter to get any colormap you want, this parameter is ignored for RGB data (images of shape (width, height, 3)). This function filters the digits (3, 9) from the dataset and randomly splits it in train and test set. """ Load data digits = load_digits() data = digits["data"] target = digits["data"] target = digits["target"] # Data filering num 1, num 2 = 3, 9 mask = np.logical_or(target == num_1, target == num_2) data = data[mask]/data.max() target = target[mask] # Relabel targets
	<pre>target[target == num_1] = -1 target[target == num_2] = 1 # split into train and test data X_all = data y_all = target X_train, X_test, y_train, y_test = model_selection.train_test_split(</pre>
In [5]:	<pre>Visualize some images to get a sense of which features might be important to distinguish the digits. fig, axes = plt.subplots(1, 4, figsize=(12, 3), tight_layout=True) index = np.random.randint(0, 100) for i in range(4): axes[i].imshow(X_train[y_train==-1][index+i].reshape(8,8), cmap="gray", interpolation="nearest") fig, axes = plt.subplots(1, 4, figsize=(12, 3), tight_layout=True) index = np.random.randint(0, 100) for i in range(4): axes[i].imshow(X_train[y_train==1][index+i].reshape(8,8), cmap="gray", interpolation="nearest")</pre>
	0-11-12-13-13-13-13-13-13-13-13-13-13-13-13-13-
In [6]:	1-2-3-3-3-3-3-3-3-3-3-3-3-3-3-3-3-3-3-3-
	<pre>input: #instances x 64 numpy array output: #instances x 2 numpy array """ images = x.reshape(-1, 8, 8) #instances x row index x column index feat1 = np.mean(images[:, 2:4, 2:4], axis=(1, 2)) feat2 = np.mean(images[:, 4:6, 4:7], axis=(1, 2)) return np.array([feat1, feat2]).T def worse_features2d(x): """ Perform a user defined dimension reduction input x: #instances x 64 numpy array output: #instances x 2 numpy array """</pre>
	<pre># mean(Image) feat1 = np.mean(x, axis=-1) # var(Image) feat2 = np.var(x, axis=-1) return np.array([feat1, feat2]).T</pre> The features2d() function looks at the average pixel values of two patches in the image. They are informative enough to more or less differentiate between the digit '3' and '9' which we can see in the scatter plot below. The worse_features2d() is much simpler and doesn't extract good features. We won't be using it for the rest of the exercise.
In [7]:	<pre>1.2 Scatter Plot def scatter_plot_simple(x, y, title="Training"): """ This function returns the dataset scatter plot input x: N x 2 numpy array input y: N x 1 numpy array output: None """ plt.figure(figsize=(8,8)) plt.gca().set_aspect('equal')</pre>
In [8]:	<pre>plt.title(title + " Scatter Plot: 3 vs 9") # Scatter plot plt.scatter(x[y == -1, 0], x[y == -1, 1], marker="o", s=30, c="b", label= "3") plt.scatter(x[y == 1, 0], x[y == 1, 1], marker="x", s=30, c="r", label= "9") plt.xlabel("feature 1") plt.ylabel("feature 2") plt.legend() plt.show()</pre> # Load data digits = load_digits()
	<pre># Dimension Reduction Xr_train, Xr_test = features2d(X_train), features2d(X_test) # Scatter Plot scatter_plot_simple(Xr_train, y_train, "Training") scatter_plot_simple(Xr_test, y_test, "Test") Training Scatter Plot: 3 vs 9</pre>
	0.6 - 0.5 - 0.5 - 0.4 - 0.4 - 0.3 - 0.4 - 0.3 - 0.5 - 0.5 - 0.5 - 0.4 - 0.3 - 0.5 -
	0.2
	0.5 - 0.5 - 0.4 - 0.4 - 0.3 - 0.3 - 0.2 - 0.2 - 0.2 - 0.5 -
In [9]:	# Dimension Reduction _Xr_train, _Xr_test = worse_features2d(X_train), worse_features2d(X_test) # Scatter Plot scatter_plot_simple(_Xr_train, y_train, "Training - Worse features") Training - Worse features Scatter Plot: 3 vs 9
	0.16 - 0.15 - 0.15 - 0.14 - 0.13 - 0.13 - 0.12 - 0.12 - 0.12 - 0.12 - 0.12 - 0.12 - 0.13 - 0.12 - 0.13 - 0.12 - 0.13 - 0.12 - 0.13 - 0.13 - 0.12 - 0.13 - 0.
In [10]:	0.11 0.26 0.28 0.30 0.32 0.34 0.36 0.38 Compute the distance of a vector x from a mean point def distance from mean(x, mean):
	Computes the L2-distance """ return np.sqrt(np.sum((x - mean[None, :])**2, axis=-1)) def nearest_mean(training_features, training_labels, test_features): """ This function returns the nearest mean predictions given input training_features: N_training x 2 numpy array input training_labels: N_training x 1 numpy array input test_features: N_test x 2 numpy array output: test_predictions: N_test numpy array """
Tn [11].	<pre>classes_list = np.unique(training_labels) mean_points = [] # Find all mean points for label in classes_list: mean_points.append(np.mean(training_features[training_labels == label], axis=0)) distance2mean = np.zeros((test_features.shape[0], classes_list.shape[0])) # Compute the distances between test_features and all mean for label in classes_list: distance2mean[:, 1*(label>0)] = distance_from_mean(test_features, mean_points[1*(label>0)]) return np.argmin(distance2mean, axis=-1)*2 - 1, mean_points</pre> # Dimension Reduction
	<pre>Xr_test = features2d(X_test) # Find Nearest Mean Predictions predicted_labels_test, mean_points = nearest_mean(Xr_train, y_train, Xr_test) predicted_labels_train, _ = nearest_mean(Xr_train, y_train, Xr_train) # Print error for test and training set print("Test error Nearest Mean: ", np.mean(predicted_labels_test != y_test)) print("Training error Nearest Mean: ", np.mean(predicted_labels_train != y_train)) Test error Nearest Mean: 0.04794520547945205 Training error Nearest Mean: 0.11059907834101383</pre>
In [12]:	Notice here that the test error is lower than the training error. This usually isn't the case, and is simply a consequence of the random samples that were drawn from the test_train_split above. If we use a different random_state, we usually will achieve a test error which is worse than the training error. def simple_linear_classifier(beta, b, test_features): """ This function returns the label as sign(x_i * beta + b) input training_features: N_training x 2 numpy array input training_labels: N_training x 1 numpy array input test_features: N_test x 2 numpy array output: test_predictions: N_test numpy array """ predicted_labels = np.sign(test_features @ beta + b) #@ = matrix multiplication in numpy return predicted_labels
In [13]:	<pre># Find good beta and b values by experimentation and comparing the error on the training data beta = np.array([0.15, -0.1]) b = -0.02 # Find Nearest Mean Predictions predicted_labels_test = simple_linear_classifier(beta, b, Xr_test) predicted_labels_train = simple_linear_classifier(beta, b, Xr_train) # Print error for test and training set print("Test error Simple Linear Classifier: ", np.mean(predicted_labels_test != y_test)) print("Training error Simple Linear Classifier: ", np.mean(predicted_labels_train != y_train)) Test error Simple Linear Classifier: 0.0547945205479452</pre>
In [15]:	<pre>Training error Simple Linear Classifier: 0.11059907834101383 2.4 Visualize the decision regions def visualization_NearestMean(Xr_train, y_train, Xr_test, y_test): """ This Function visualizes the decision regions for the Nearest Mean Classifier """ # Build Grid feat_min, feat_max = np.min(Xr_test, axis=0), np.max(Xr_test, axis=0) x, y = np.linspace(feat_min[0], feat_max[0], 2000), np.linspace(feat_max[1], feat_min[1], 2000) xx = np.array(np.meshgrid(x, y)).reshape(2, -1).T # meshgrid produces a 2x2 array with tuples of x</pre>
	<pre># Predict grid labels predicted_labels, mean_points = nearest_mean(Xr_train, y_train, xx) # Decison boundary plt.figure(figsize=(8,8)) plt.gca().set_aspect('equal') plt.title("Decision Regions for Nearest Mean Classifier (Blue: 3, Red: 9)") plt.imshow(((predicted_labels>0)*1).reshape(-1, 2000),</pre>
	<pre>plt.scatter(Xr_test[y_test == -1, 0], Xr_test[y_test == -1, 1], marker="o", s=30, c="b", label= "3" plt.scatter(Xr_test[y_test == 1, 0], Xr_test[y_test == 1, 1], marker="x", s=30, c="r", label= "9") # Scatter mean points plt.scatter(mean_points[0][0], mean_points[0][1], marker="o", s=50, c="g", label= "Mean") plt.scatter(mean_points[1][0], mean_points[1][1], marker="o", s=50, c="g") plt.xlim(feat_min[0], feat_max[0]) plt.ylim(feat_min[1], feat_max[1]) plt.xlabel("feature 1") plt.ylabel("feature 2") plt.legend() plt.show()</pre>
In [16]:	Decision Regions for Nearest Mean Classifier (Blue: 3, Red: 9) 0.6 -
	0.4 0.5 0.4 0.6 0.8 × × × × × × × × × × × × × × × × × × ×
In [19]:	<pre>def visualization_SimpleLinearClassifier(beta, b, Xr_test, y_test): """ This Function visualizes the decision regions for the Simple Linear Classifier """ # Build Grid feat_min, feat_max = np.min(Xr_test, axis=0), np.max(Xr_test, axis=0) x, y = np.linspace(feat_min[0], feat_max[0], 2000), np.linspace(feat_max[1], feat_min[1], 2000) xx = np.array(np.meshgrid(x, y)).reshape(2, -1).T # Predict grid labels predicted_labels = simple_linear_classifier(beta, b, xx)</pre>
	<pre># Decison boundary plt.figure(figsize=(8,8)) plt.gca().set_aspect('equal') plt.title("Decision Regions for Simple Linear Classifier (Blue: 3, Red: 9)") plt.imshow(((predicted_labels>0)*1).reshape(-1, 2000),</pre>
In [20]:	<pre>plt.xlim(feat_min[0], feat_max[0]) plt.ylim(feat_min[1], feat_max[1]) plt.xlabel("feature 1") plt.ylabel("feature 2") plt.legend() plt.show() visualization_SimpleLinearClassifier(beta, b, Xr_test, y_test) Decision Regions for Simple Linear Classifier (Blue: 3, Red: 9) x</pre>
	0.6 -
In [21]:	This function computes for each class: mean and priors, and the global covariance matrix input training_features: N_training x 2 numpy array input training_labels: N_training x 1 numpy array
	<pre>input training_labels: N_training x 1 numpy array output lists of means, covariances and priors """ mu, cov, p = [], [], [] for label in np.unique(training_labels): # filtering the correct class data = training_features[training_labels == label] # mean mean = np.mean(data, axis=0) mu.append(mean) # Priors p.append(data.shape[0]/training_features.shape[0]) # Global Variance, subtract class means first</pre>
In [22]:	<pre>global_feat = training_features - np.array(mu)[training_labels] cov = np.dot(global_feat.T, global_feat)/training_features.shape[0] return mu, cov, p 3.2 Implement LDA Prediction def predict_lda(mu, cov, p, test_features): """ This function returns the LDA predictions given as input lists of means, priors and the global covariance matrix input test_features: N_test x 2 numpy array</pre>
In [23]:	<pre>output: test_predictions: N_test numpy array """ beta = np.linalg.inv(cov) @ (mu[1] - mu[0]).T b = -1/2*(mu[0] + mu[1]) @ beta + np.log(p[1]/p[0]) predicted_labels = np.sign(test_features @ beta + b) return predicted_labels # Fit LDA mu, cov, p = fit_lda(Xr_train, y_train) # Find LDA Predictions predicted_labels_test = predict_lda(mu, cov, p, Xr_test)</pre>
т	predicted_labels_train = predict_lda(mu, cov, p, Xr_train) # Print error rates print("Test error LDA: ", np.mean(predicted_labels_test != y_test)) print("Training error LDA: ", np.mean(predicted_labels_train != y_train)) Test error LDA: 0.0684931506849315 Training error LDA: 0.11059907834101383 Now we apply LDA to the full data i.e. we have 64 features instead of 2. As there are pixels which are always off (e.g. in the corners) the covariance matrix will have a zero determinant and it won't be possible to calculate the inverse for the prediction. Thus we first filter out the pixels which have a very low variance.
[24]:	<pre># Fit LDA on full pixel vectors vars = np.var(X_train, axis=0) mask = (vars>0.001) print('Number of remaining dimensions:', np.sum(mask)) x_test_clean = X_test[:, mask] x_train_clean = X_train[:, mask] mu_full, cov_full, p_full = fit_lda(x_train_clean, y_train) print('Determinant of covariance matrix:', np.linalg.det(cov_full)) # The determinant of the full covar iance matrix has to be non-zero # Find LDA Predictions predicted_labels_test = predict_lda(mu_full, cov_full, p_full, x_test_clean) predicted_labels_train = predict_lda(mu_full, cov_full, p_full, x_train_clean)</pre>
	# Print error rates print("Test error LDA: ", np.mean(predicted_labels_test != y_test)) print("Training error LDA: ", np.mean(predicted_labels_train != y_train)) Number of remaining dimensions: 47 Determinant of covariance matrix: 1.08807662182273e-79 Test error LDA: 0.0 Training error LDA: 0.004608294930875576 mu_full is a 2-tuple of 64-dim vectors and cov_full is a 64x64 matrix. In total we have 2 * 64 + 64 * 64 = 4224 parameters to "train". As our dataset only consists of 363 images (only '3' and '9' digits) this model can, from an information theory point of view, memorize the entire
In [29]:	dataset and we achive a training error of nearly zero. For comparatively low-dimensional data like the 64 pixel images, it is feasible to train on the all dimensions of the input, but for higher-dimensional data and larger datasets it is usually necessary to use some kind of dimensionality reduction. 3.3 Visualization def plot_ellipse_axis(mu, cov, color="blue"): """ This function plots the main axis of the distribution given mean and covariance matrix """ # Eigenvalues/Eigenvector decomposition [lamb1, lamb2], [vec_1, vec_2] = np.linalg.eig(cov)
	<pre>[lamb1, lamb2], [vec_1, vec_2] = np.linalg.eig(cov) lamb1, lamb2 = np.sqrt(lamb1), np.sqrt(lamb2) # Plot axis 1 x1, y1 = ([mu[0] - lamb1*vec_1[0], mu[0] + lamb1*vec_1[0]],</pre>
	This Function visualizes the decision regions for the LDA Classifier """ # Build Grid feat_min, feat_max = np.min(Xr_test, axis=0), np.max(Xr_test, axis=0) x, y = np.linspace(feat_min[0], feat_max[0], 200), np.linspace(feat_max[1], feat_min[1], 200) xx = np.array(np.meshgrid(x, y)).reshape(2, -1).T # Predict grid labels predicted_labels = predict_lda(mu, cov, p, xx) plt.figure(figsize=(8,8)) plt.gca().set_aspect('equal') plt.title("Decision Regions (Blue: 3, Red: 9)")
	<pre>plt.title("Decision Regions (Blue: 3, Red: 9)") plt.imshow(((predicted_labels>0)*1).reshape(-1, 200),</pre>
In [30]:	<pre>plot_ellipse_axis(mu[0], cov, color="blue") plot_ellipse_axis(mu[1], cov, color="red") plt.xlim(feat_min[0], feat_max[0]) plt.ylim(feat_min[1], feat_max[1]) plt.xlabel("feature 1") plt.ylabel("feature 2") plt.legend() plt.show() # Visualize training data visualization_LDA(Xr_train, y_train, mu, cov, p)</pre> Decision Regions (Blue: 3, Red: 9)
	Decision Regions (Blue: 3, Red: 9) 0.7 0.6 0.7 0.7 0.8 0.9 0.9 0.9 0.9 0.9 0.9 0.9
	0.2 0.4 0.6 0.8 Notice here that the axes of both clusters are the same, as LDA uses the same covariance matrix for each class. 3.4 Quantitative performance evaluation
In [31]:	<pre>from sklearn.model_selection import KFold def cross_validation(digits, fit_func, pred_func, num_sample=10): """ Measure the correct accuracy with cross validation """ # Get data data = digits["data"] target = digits["target"] # Need to prepare data again since 'data_preparation' returns test - train split # Data filering num_1, num_2 = 3, 9 mask = np.logical_or(target == num_1, target == num_2)</pre>
	<pre>mask = np.logical_or(target == num_1, target == num_2) data = data[mask]/data.max() target = target[mask] # Delete dead pixels vars = np.var(data, axis=0) mask = (vars>0.001) data = data[:, mask] # Relabel targets target[target == num_1] = -1 target[target == num_2] = 1 # Splits k_folds = KFold(n_splits=num_sample) # This creates a "KFold object" from the sklearn library, with</pre>
In ¹	
ın [32]:	# Digits digits = load_digits() # Print Cross validation accuracy cross_validation(digits, fit_lda, predict_lda, 10) Mean Error Rate with Cross Validation: 0.013739 +/- 0.025530 As k-fold cross validation performs multiple error estimations, it is less prone to statistical occurences like above, where due to the random selection of instances by chance resulted in the test error being lower than the training error, which usually is not the case statistically speaking. 4 SVM
In [33]:	<pre>def predict_SVM(beta, b, test_features): """ This function returns the SVM predictions given as input beta and b input test_features: N_test x 2 numpy array output: test_predictions: N_test numpy array """ predicted_labels = np.sign(test_features @ beta + b) return predicted_labels</pre>

In [34]:	<pre>input training input 1: float output beta, """ # Initial gue beta = np.rand b = 0 def ReLU(x): return np</pre>	ing_features, traing_features: N_traing_labels: N_training_labels: N_training_labels: N_training_labels: N_training_t, T: int, tau: floods, List of Loss and both search and both dom.normal(loc=0, search). where(x>0, x, 0)	ning x N_feature ng x 1 numpy ar. oat d train_error	es numpy array ray					
	Loss = [] train_error = [] N = len(training_labels) # Implement training loop using the gradient descent algorithm for i in range(T): # Helper variable temp = training_labels*(training_features @ beta + b) # Compute Loss Loss.append(1/2*np.dot(beta, beta) + 1*np.mean(ReLU(1 - temp))) # Compute training error at each iteration with current guess of beta and b predicted_labels_train = predict_SVM(beta, b, training_features) train_error.append(np.mean(predicted_labels_train != training_labels)) # Compute gradients of beta and b grad_beta = beta + 1*np.mean(np.where(temp[:,None] < 1, -training_labels[:, None]*training_features, 0), axis=0) grad_b = 1*np.mean(np.where(temp < 1, -training_labels, 0))								
In [43]:	grad_beta ures, 0), axis=0) grad_b = 1 # Update beta = beta b = b - ta return beta, b # Fit SVM with had beta, b, Loss, tra # Print beta and if print('beta =', beta print('b =', b) beta = [4.2068992]	= beta + l*np.mean l*np.mean(np.where current guess of beta ta - tau*grad_beta au*grad_b b, Loss, train_erro nd-picked hyperpara ain_error = fit_SVI b eta) 25 -1.58718237]	n(np.where(temp (temp < 1, -tra: eta and b or ameters	ining_labels, 0))		y_feat		
In [44]:	<pre>b = -1.09861751152 # Visualizations visualization_Simple</pre>	207266			* * * * * * *	3 9			
In [45]:	<pre># Find SVM Predic predicted_labels_t predicted_labels_t # Print error rate print("Test error print("Training extended to the companion of the companion o</pre>	<i>tions</i> test = predict_SVM train = predict_SVM	feature 1 (beta, b, Xr_team) M(beta, b, Xr_team) redicted_labels an (predicted_labels)	st) cain) _test != y_test))				
In [53]:	plt.figure(figsize plt.title('Loss as plt.plot(Loss) plt.xlabel('T') plt.grid() plt.show()		Loss after T	steps					
	90								
In [54]:	plt.figure(figsize plt.title('Training plt.plot(train_er: plt.xlabel('T') plt.grid() plt.show()	ng error after T st	400 T	600	800	1000			
	0.6	Tra	aining error afte	er T steps					
	0.3	200	400 T	600	800	1000			
In [55]:	<pre>def cross_validat: """ Measure the co """ # Iterate thro for 1 in lambo # Splits k_folds = mean_rate for i, (trees.)</pre>	<pre>l_selection import ion_SVM(X_train, y_ orrect accuracy wi ough all parameter. das: KFold(n_splits=nur = np.zeros(num_sar rain, test) in enur b, _, _ = fit_SVM</pre>	_train, lambdas= th cross valida s m_sample) mple) mple) merate(k_folds.s	tion for a given	n list of hyp	perparameters (1	ambdas)		
In [56]:	predicted_labels = predict_SVM(beta, b, X_train[test]) mean_rate[i] = np.mean(predicted_labels != y_train[test]) print("Mean Error Rate with Cross Validation for lambda=%f: %f +/- %f"%(l,np.mean(mean_rate), p.std(mean_rate))) 56]: cross_validation_SVM(Xr_train, y_train, lambdas=[1,10,100,1e3,1e4,1e5], T=1000, tau=0.001, num_sample: 0) Mean Error Rate with Cross Validation for lambda=1.000000: 0.567316 +/- 0.128417 Mean Error Rate with Cross Validation for lambda=10.000000: 0.362771 +/- 0.131922 Mean Error Rate with Cross Validation for lambda=100.000000: 0.115584 +/- 0.056693 Mean Error Rate with Cross Validation for lambda=1000.000000: 0.151515 +/- 0.056150 Mean Error Rate with Cross Validation for lambda=10000.000000: 0.151515 +/- 0.079157 Mean Error Rate with Cross Validation for lambda=10000.000000: 0.197619 +/- 0.137159								
In [57]:	# Fit SVM on full beta, b, Loss, tra # Find SVM Predicted_labels_tended_	If with $\lambda=100~{ m or}~1000$ is the full pixel vector. The full pixel vector. The full pixel vector is sufficient to some state of the full pixel vector. The full pixel vector is sufficient to some suff	M(X_train, y_train) (beta, b, X_test) M(beta, b, X_train) redicted_labels	ain, l=100, T=10 t) ain) test != y_test)	000, tau=0.00				
In [58]:	Test error SVM: (Training error SVM cross_validation_s) Mean Error Rate was Mean E	4: 0.009216589861 ⁻	in, lambdas=[1,2] on for lambda=1;	.000000: 0.40800 0.000000: 0.0415 00.000000: 0.013 000.000000: 0.02	De5], T=1000, 09 +/- 0.2365 058 +/- 0.038 058853 +/- 0.02 022944 +/- 0.0 018398 +/- 0.	74 377 1168 22952 022541	_sample=10		