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1 import matplotlib.pyplot as plt
2 import numpy as np
3 import os
4
5 PLOT_COLORS = ['red', 'green', 'blue', 'orange'] # Colors for your plots
6 K = 4 # Number of Gaussians in the mixture model
7 NUM_TRIALS = 3 # Number of trials to run (can be adjusted for debugging)
8 UNLABELED = -1 # Cluster label for unlabeled data points (do not change)
9
10
11 def main(is_semi_supervised, trial_num):
12     """Problem 3: EM for Gaussian Mixture Models (unsupervised and semi-supervised)"""
13     print('Running {} EM algorithm...'
14           .format('semi-supervised' if is_semi_supervised else 'unsupervised'))
15
16     # Load dataset
17     train_path = os.path.join('.', 'train.csv')
18     x_all, z_all = load_gmm_dataset(train_path)
19
20     # Split into labeled and unlabeled examples
21     labeled_idx = (z_all != UNLABELED).squeeze()
22     x_tilde = x_all[labeled_idx, :] # Labeled examples
23     z_tilde = z_all[labeled_idx, :] # Corresponding labels
24     x = x_all[~labeled_idx, :] # Unlabeled examples
25
26     # *** START CODE HERE ***
27     # (1) Initialize mu and sigma by splitting the n_examples data points uniformly at random
28     # into K groups, then calculating the sample mean and covariance for each group
29     n, d = x.shape
30     group = np.random.choice(K, n)
31     mu = [np.mean(x[group == g, :], axis=0) for g in range(K)]
32     sigma = [np.cov(x[group == g, :].T) for g in range(K)]
33
34     # (2) Initialize phi to place equal probability on each Gaussian
35     # phi should be a numpy array of shape (K,)
36     phi = np.full((K,), fill_value=(1. / K), dtype=np.float32)
37
38     # (3) Initialize the w values to place equal probability on each Gaussian
39     # w should be a numpy array of shape (n, K)
40     w = np.full((n, K), fill_value=(1. / K), dtype=np.float32)
41     # *** END CODE HERE ***
42
43     if is_semi_supervised:
44         w = run_semi_supervised_em(x, x_tilde, z_tilde, w, phi, mu, sigma)
45     else:
46         w = run_em(x, w, phi, mu, sigma)
47
48     # Plot your predictions
49     z_pred = np.zeros(n)
50     if w is not None: # Just a placeholder for the starter code
51         for i in range(n):
52             z_pred[i] = np.argmax(w[i])
53
54     plot_gmm_preds(x, z_pred, is_semi_supervised, plot_id=trial_num)
55
56
57 def run_em(x, w, phi, mu, sigma):
58     """Problem 3(d): EM Algorithm (unsupervised).
59
60     See inline comments for instructions.
61
62     Args:
63         x: Design matrix of shape (n_examples, dim).
64         w: Initial weight matrix of shape (n_examples, k).
65         phi: Initial mixture prior, of shape (k,).
66         mu: Initial cluster means, list of k arrays of shape (dim,).
67         sigma: Initial cluster covariances, list of k arrays of shape (dim, dim).
68
69     Returns:
70         Updated weight matrix of shape (n_examples, k) resulting from EM algorithm.
71         More specifically, w[i, j] should contain the probability of
72         example x^(i) belonging to the j-th Gaussian in the mixture.

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73 """
74 # No need to change any of these parameters
75 eps = 1e-3 # Convergence threshold
76 max_iter = 1000
77
78 # Stop when the absolute change in log-likelihood is < eps
79 # See below for explanation of the convergence criterion
80 it = 0
81 ll = prev_ll = None
82 while it < max_iter and (prev_ll is None or np.abs(ll - prev_ll) >= eps):
83     pass # Just a placeholder for the starter code
84     # *** START CODE HERE
85     # (1) E-step: Update your estimates in w
86     w = e_step(x, w, phi, mu, sigma)
87
88     # (2) M-step: Update the model parameters phi, mu, and sigma
89     phi, mu, sigma = m_step(x, w, mu, sigma)
90
91     # (3) Compute the log-likelihood of the data to check for convergence.
92     # By log-likelihood, we mean `ll = sum_x[log(sum_z[p(x|z) * p(z)])]`.
93     # We define convergence by the first iteration where abs(ll - prev_ll) < eps.
94     # Hint: For debugging, recall part (a). We showed that ll should be monotonically increasing.
95     prev_ll = ll
96     ll = log_likelihood(x, phi, mu, sigma)
97     it += 1
98     print('[iter: {:03d}, log-likelihood: {:.4f}]'.format(it, ll))
99     # *** END CODE HERE ***
100
101 return w
102
103
104 def run_semi_supervised_em(x, x_tilde, z_tilde, w, phi, mu, sigma):
105     """Problem 3(e): Semi-Supervised EM Algorithm.
106
107     See inline comments for instructions.
108
109     Args:
110         x: Design matrix of unlabeled examples of shape (n_examples_unobs, dim).
111         x_tilde: Design matrix of labeled examples of shape (n_examples_obs, dim).
112         z_tilde: Array of labels of shape (n_examples_obs, 1).
113         w: Initial weight matrix of shape (n_examples, k).
114         phi: Initial mixture prior, of shape (k,).
115         mu: Initial cluster means, list of k arrays of shape (dim,).
116         sigma: Initial cluster covariances, list of k arrays of shape (dim, dim).
117
118     Returns:
119         Updated weight matrix of shape (n_examples, k) resulting from semi-supervised EM algorithm.
120         More specifically, w[i, j] should contain the probability of
121         example x^(i) belonging to the j-th Gaussian in the mixture.
122     """
123     # No need to change any of these parameters
124     alpha = 20. # Weight for the labeled examples
125     eps = 1e-3 # Convergence threshold
126     max_iter = 1000
127
128     # Stop when the absolute change in log-likelihood is < eps
129     # See below for explanation of the convergence criterion
130     it = 0
131     ll = prev_ll = None
132     while it < max_iter and (prev_ll is None or np.abs(ll - prev_ll) >= eps):
133         pass # Just a placeholder for the starter code
134         # *** START CODE HERE ***
135         # (1) E-step: Update your estimates in w
136         w = e_step(x, w, phi, mu, sigma)
137
138         # (2) M-step: Update the model parameters phi, mu, and sigma
139         phi, mu, sigma = m_step_ss(x, x_tilde, z_tilde, w, phi, mu, sigma, alpha)
140
141         # (3) Compute the log-likelihood of the data to check for convergence.
142         # Hint: Make sure to include alpha in your calculation of ll.
143         # Hint: For debugging, recall part (a). We showed that ll should be monotonically increasing.
144         prev_ll = ll

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145     ll = log_likelihood(x, phi, mu, sigma)
146     ll += alpha * log_likelihood(x_tilde, phi, mu, sigma, z_tilde)
147     it += 1
148     print('[iter: {:03d}, log-likelihood: {:.4f}'].format(it, ll))
149     # *** END CODE HERE ***
150
151     return w
152
153
154 # *** START CODE HERE ***
155 # Helper functions
156
157 def e_step(x, w, phi, mu, sigma):
158     """E-step for both unsupervised and semi-supervised EM."""
159     n, d = x.shape
160     k = len(mu)
161
162     for i in range(n):
163         for j in range(k):
164             w[i, j] = p_x_given_z(x[i], mu[j], sigma[j]) * phi[j]
165
166     w /= np.sum(w, axis=1, keepdims=True)
167
168     return w
169
170
171 def m_step(x, w, mu, sigma):
172     """M-step for unsupervised EM."""
173     n, d = x.shape
174     k = len(mu)
175
176     phi = np.mean(w, axis=0)
177
178     for j in range(k):
179         w_j = w[:, j:j + 1]
180         mu[j] = np.sum(w_j * x, axis=0) / np.sum(w_j)
181
182         sigma[j] = np.zeros_like(sigma[j])
183         for i in range(n):
184             x_minus_mu = x[i] - mu[j]
185             sigma[j] += w[i, j] * np.outer(x_minus_mu, x_minus_mu)
186         sigma[j] /= np.sum(w_j)
187
188     return phi, mu, sigma
189
190
191 def m_step_ss(x, x_tilde, z_tilde, w, phi, mu, sigma, alpha):
192     """M-step for semi-supervised EM."""
193     n, _ = x.shape
194     n_tilde, _ = x_tilde.shape
195     k = len(mu)
196
197     w_colsums = np.sum(w, axis=0)
198     k_counts = [np.sum(z_tilde == j) for j in range(k)]
199     for j in range(k):
200         phi[j] = (w_colsums[j] + alpha * k_counts[j]) / (n + alpha * n_tilde)
201
202         w_j = w[:, j:j + 1]
203         mu[j] = ((np.sum(w_j * x, axis=0)
204                  + alpha * np.sum(x_tilde[(z_tilde == j).squeeze(), :], axis=0))
205                  / (np.sum(w_j) + alpha * k_counts[j]))
206
207         sigma[j] = np.zeros_like(sigma[j])
208         for i in range(n):
209             x_minus_mu = x[i] - mu[j]
210             sigma[j] += w[i, j] * np.outer(x_minus_mu, x_minus_mu)
211         for i in range(n_tilde):
212             if z_tilde[i] == j:
213                 x_minus_mu = x_tilde[i] - mu[j]
214                 sigma[j] += alpha * np.outer(x_minus_mu, x_minus_mu)
215         sigma[j] /= (np.sum(w_j) + alpha * k_counts[j])
216

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217     return phi, mu, sigma
218
219
220 def log_likelihood(x, phi, mu, sigma, z=None):
221     """Get log-likelihood of the data `x` given model parameters
222     `phi`, `mu`, and `sigma`.
223     """
224     n, d = x.shape
225     k = len(phi)
226     ll = 0.
227     for i in range(n):
228         if z is None: # Unsupervised case
229             p_x = 0.
230             for j in range(k):
231                 p_x += p_x_given_z(x[i], mu[j], sigma[j]) * phi[j]
232         else: # Supervised case
233             j = int(z[i])
234             p_x = p_x_given_z(x[i], mu[j], sigma[j]) * phi[j]
235         ll += np.log(p_x)
236
237     return ll
238
239
240 def p_x_given_z(x, mu, sigma):
241     """Get probability of a single example `x` given model parameters
242     `mu` and `sigma` (corresponding to cluster  $z = j$ ).
243     """
244     d = len(x)
245     assert d == len(mu) and sigma.shape == (d, d), 'Shape mismatch.'
246
247     c = 1. / ((2. * np.pi) ** (d / 2) * np.sqrt(np.linalg.det(sigma)))
248     x_minus_mu = x - mu
249     sigma_inv = np.linalg.inv(sigma)
250     p_val = c * np.exp(-.5 * x_minus_mu.dot(sigma_inv).dot(x_minus_mu.T))
251
252     return p_val
253 # *** END CODE HERE ***
254
255
256 def plot_gmm_preds(x, z, with_supervision, plot_id):
257     """Plot GMM predictions on a 2D dataset `x` with labels `z`.
258
259     Write to the output directory, including `plot_id`
260     in the name, and appending `ss` if the GMM had supervision.
261
262     NOTE: You do not need to edit this function.
263     """
264     plt.figure(figsize=(12, 8))
265     plt.title('{} GMM Predictions'.format('Semi-supervised' if with_supervision else 'Unsupervised'))
266     plt.xlabel('x_1')
267     plt.ylabel('x_2')
268
269     for x_1, x_2, z_ in zip(x[:, 0], x[:, 1], z):
270         color = 'gray' if z_ < 0 else PLOT_COLORS[int(z_)]
271         alpha = 0.25 if z_ < 0 else 0.75
272         plt.scatter(x_1, x_2, marker='.', c=color, alpha=alpha)
273
274     file_name = 'pred{}_{}.pdf'.format('_ss' if with_supervision else '', plot_id)
275     save_path = os.path.join('.', file_name)
276     plt.savefig(save_path)
277
278
279 def load_gmm_dataset(csv_path):
280     """Load dataset for Gaussian Mixture Model.
281
282     Args:
283         csv_path: Path to CSV file containing dataset.
284
285     Returns:
286         x: NumPy array shape (n_examples, dim)
287         z: NumPy array shape (n_examples, 1)
288

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289 NOTE: You do not need to edit this function.
290 """
291
292 # Load headers
293 with open(csv_path, 'r') as csv_fh:
294     headers = csv_fh.readline().strip().split(',')
295
296 # Load features and labels
297 x_cols = [i for i in range(len(headers)) if headers[i].startswith('x')]
298 z_cols = [i for i in range(len(headers)) if headers[i] == 'z']
299
300 x = np.loadtxt(csv_path, delimiter=',', skiprows=1, usecols=x_cols, dtype=float)
301 z = np.loadtxt(csv_path, delimiter=',', skiprows=1, usecols=z_cols, dtype=float)
302
303 if z.ndim == 1:
304     z = np.expand_dims(z, axis=-1)
305
306 return x, z
307
308
309 if __name__ == '__main__':
310     np.random.seed(229)
311     # Run NUM_TRIALS trials to see how different initializations
312     # affect the final predictions with and without supervision
313     for t in range(NUM_TRIALS):
314         main(is_semi_supervised=False, trial_num=t)
315
316         # *** START CODE HERE ***
317         # Once you've implemented the semi-supervised version,
318         # uncomment the following line.
319         # You do not need to add any other lines in this code block.
320
321         # main(is_semi_supervised=True, trial_num=t)
322
323         # *** END CODE HERE ***

```