

Machine Learning HW2

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November 20, 2025

Usage of Artificial Intelligence Tools

In this homework, I utilized my code in HW 1, which was developed without AI assistance. The code for PCA implementation and plotting was written by myself, based on my understanding of the concepts.

For the report, to make my expression more academic and formal, I used ChatGPT to help refine and polish the language in certain sections of the report. Besides, I utilized ChatGPT to help me generate the plots due to unfamiliarity with the matplotlib library. I provided ChatGPT with my original text and requested suggestions for improvement, which I then reviewed and incorporated as appropriate.

Code Structure

The file `numpy_accr.py` contains the main implementation of PCA and LOOCV evaluation. The file `plot.py` is used for generating the required plots. It's modified from `numpy_accr.py`, so the functions may be similar.

The file `multi_core_accr.py` integrates multiprocessing optimizations for LOOCV to further enhance computational efficiency.

Parallel processing may not be supported in all environments (the experiments were conducted on Ubuntu 24.04.3 LTS with Linux kernel 6.14.0-33-generic, Python 3.10.13). Therefore, a NumPy-optimized version is also provided for compatibility. If the environment supports multiprocessing, it is recommended to execute the multi-core accelerated version, which produces results within only a few seconds.

1. (a) I decided to use Proportion of Variance (PoV) with $\text{thresh} = 0.95$ to determine the number of principal components to keep. With this threshold, I found that each fold selected 7 principal components to retain at least 95% of the variance in the data. This may be caused by the characteristics of loocv, where each training fold is very similar to the overall dataset, leading to consistent PCA results across folds. The execution log for PCA in each fold is provided in Appendix A.
- (b) The overall performance of Bayesian classification with PCA ($\text{thresh}=0.95$) using LOOCV is summarized in Table 1 below, and the confusion matrix is shown in Table 2. Fig. 1 presents the ROC curve for this configuration.

Metric	Value
Accuracy	0.8835
Precision	0.8421
Recall (Sensitivity)	0.8537
Specificity	0.9032
AUC	0.9256

Table 1: LOOCV Performance with PCA ($\text{thresh}=0.95$)

Confusion Matrix	Positive	Negative
True Predict	35(TP)	56(TN)
False Predict	6(FP)	6(FN)

Table 2: LOOCV Confusion Matrix with PCA ($\text{thresh}=0.95$)

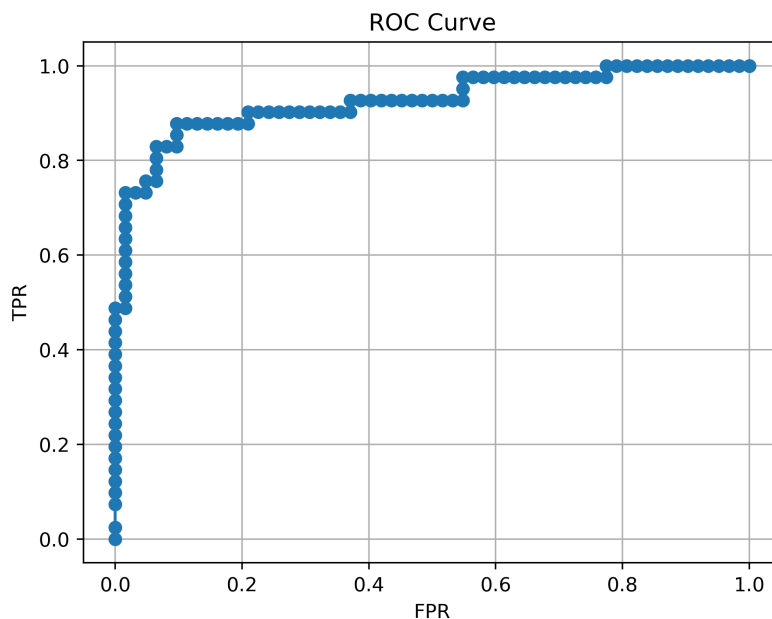


Figure 1: LOOCV ROC Curve with PCA (thresh=0.95)

With the execution results above, we can see that applying PCA with a variance retention threshold of 95% leads to a robust classification performance. The AUC of 0.9256 indicates a strong ability to distinguish between the positive and negative classes. The accuracy of 88.35% further supports the effectiveness of this approach in the given dataset.

However, the limited amount of data may lead to overfitting. This high performance might not generalize well to unseen data. Although this method performs well on the current dataset under LOOCV evaluation, it still needs further validation on larger and more diverse datasets to confirm its robustness and generalizability.

2. (a) The PCA scree plot is shown in Fig. 2.

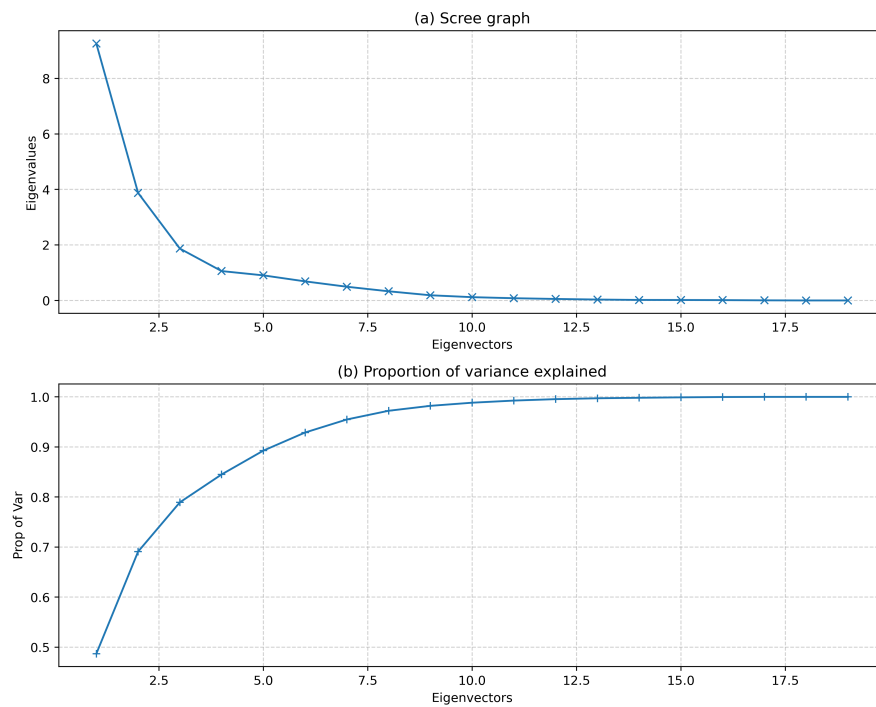


Figure 2: PCA Scree Plot

- (b) The top 5 eigenvalues are: 9.254088, 3.874613, 1.869370, 1.058813, and 0.904257. All eigenvalues and their corresponding eigenvectors can be found in Appendix B.
- (c) PCA projection with Gaussian contours and decision boundary is shown in Fig. 3.

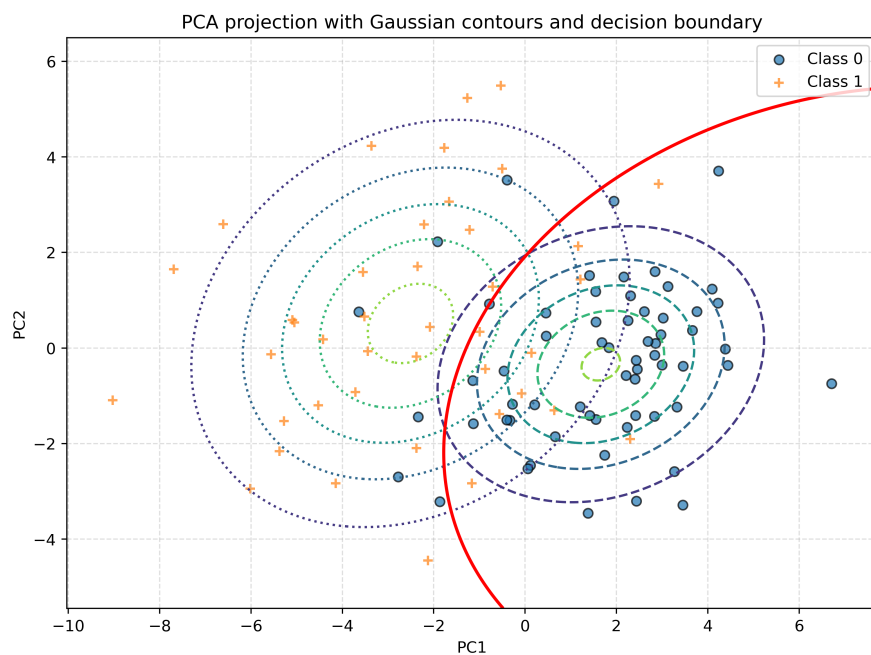


Figure 3: PCA 2D Projection with Gaussian Contours and Decision Boundary

A PCA execution log

Following is the log messages printed during PCA execution in each LOOCV fold.

```
1 [INFO] Starting Leave-One-Out Cross-Validation...
2 start with thresh=0.95
3 LOOCV Fold 1/103
4 [INFO] selected 7 principal components to retain 95.39% variance.
5 Fold 1 Training AUC: 0.9572
6 Fold 1 Test Posterior: 0.0000 (True Label: 0)
7 LOOCV Fold 2/103
8 [INFO] selected 7 principal components to retain 95.47% variance.
9 Fold 2 Training AUC: 0.9600
10 Fold 2 Test Posterior: 0.8823 (True Label: 0)
11 LOOCV Fold 3/103
12 [INFO] selected 7 principal components to retain 95.48% variance.
13 Fold 3 Training AUC: 0.9572
14 Fold 3 Test Posterior: 0.0272 (True Label: 0)
15 LOOCV Fold 4/103
16 [INFO] selected 7 principal components to retain 95.48% variance.
17 Fold 4 Training AUC: 0.9556
18 Fold 4 Test Posterior: 0.0003 (True Label: 0)
19 LOOCV Fold 5/103
20 [INFO] selected 7 principal components to retain 95.43% variance.
21 Fold 5 Training AUC: 0.9568
22 Fold 5 Test Posterior: 0.0001 (True Label: 0)
23 LOOCV Fold 6/103
24 [INFO] selected 7 principal components to retain 95.48% variance.
25 Fold 6 Training AUC: 0.9568
26 Fold 6 Test Posterior: 0.2732 (True Label: 0)
27 LOOCV Fold 7/103
28 [INFO] selected 7 principal components to retain 95.48% variance.
29 Fold 7 Training AUC: 0.9564
30 Fold 7 Test Posterior: 0.0004 (True Label: 0)
31 LOOCV Fold 8/103
32 [INFO] selected 7 principal components to retain 95.46% variance.
33 Fold 8 Training AUC: 0.9572
34 Fold 8 Test Posterior: 0.0102 (True Label: 0)
35 LOOCV Fold 9/103
36 [INFO] selected 7 principal components to retain 95.52% variance.
37 Fold 9 Training AUC: 0.9548
38 Fold 9 Test Posterior: 0.0246 (True Label: 0)
39 LOOCV Fold 10/103
40 [INFO] selected 7 principal components to retain 95.50% variance.
41 Fold 10 Training AUC: 0.9576
42 Fold 10 Test Posterior: 0.6959 (True Label: 0)
43 LOOCV Fold 11/103
44 [INFO] selected 7 principal components to retain 95.49% variance.
45 Fold 11 Training AUC: 0.9584
46 Fold 11 Test Posterior: 0.8634 (True Label: 0)
47 LOOCV Fold 12/103
48 [INFO] selected 7 principal components to retain 95.51% variance.
49 Fold 12 Training AUC: 0.9572
50 Fold 12 Test Posterior: 0.9936 (True Label: 0)
51 LOOCV Fold 13/103
52 [INFO] selected 7 principal components to retain 95.52% variance.
53 Fold 13 Training AUC: 0.9580
```

```
54 Fold 13 Test Posterior: 0.2064 (True Label: 0)
55 LOOCV Fold 14/103
56 [INFO] selected 7 principal components to retain 95.51% variance.
57 Fold 14 Training AUC: 0.9552
58 Fold 14 Test Posterior: 0.0250 (True Label: 0)
59 LOOCV Fold 15/103
60 [INFO] selected 7 principal components to retain 95.47% variance.
61 Fold 15 Training AUC: 0.9548
62 Fold 15 Test Posterior: 0.0057 (True Label: 0)
63 LOOCV Fold 16/103
64 [INFO] selected 7 principal components to retain 95.53% variance.
65 Fold 16 Training AUC: 0.9560
66 Fold 16 Test Posterior: 0.0031 (True Label: 0)
67 LOOCV Fold 17/103
68 [INFO] selected 7 principal components to retain 95.49% variance.
69 Fold 17 Training AUC: 0.9552
70 Fold 17 Test Posterior: 0.0002 (True Label: 0)
71 LOOCV Fold 18/103
72 [INFO] selected 7 principal components to retain 95.49% variance.
73 Fold 18 Training AUC: 0.9556
74 Fold 18 Test Posterior: 0.2335 (True Label: 0)
75 LOOCV Fold 19/103
76 [INFO] selected 7 principal components to retain 95.50% variance.
77 Fold 19 Training AUC: 0.9548
78 Fold 19 Test Posterior: 0.0165 (True Label: 0)
79 LOOCV Fold 20/103
80 [INFO] selected 7 principal components to retain 95.49% variance.
81 Fold 20 Training AUC: 0.9552
82 Fold 20 Test Posterior: 0.0008 (True Label: 0)
83 LOOCV Fold 21/103
84 [INFO] selected 7 principal components to retain 95.57% variance.
85 Fold 21 Training AUC: 0.9556
86 Fold 21 Test Posterior: 0.0003 (True Label: 0)
87 LOOCV Fold 22/103
88 [INFO] selected 7 principal components to retain 95.51% variance.
89 Fold 22 Training AUC: 0.9568
90 Fold 22 Test Posterior: 0.0194 (True Label: 0)
91 LOOCV Fold 23/103
92 [INFO] selected 7 principal components to retain 95.50% variance.
93 Fold 23 Training AUC: 0.9560
94 Fold 23 Test Posterior: 0.0602 (True Label: 0)
95 LOOCV Fold 24/103
96 [INFO] selected 7 principal components to retain 95.51% variance.
97 Fold 24 Training AUC: 0.9568
98 Fold 24 Test Posterior: 0.0205 (True Label: 0)
99 LOOCV Fold 25/103
100 [INFO] selected 7 principal components to retain 95.54% variance.
101 Fold 25 Training AUC: 0.9556
102 Fold 25 Test Posterior: 0.0366 (True Label: 0)
103 LOOCV Fold 26/103
104 [INFO] selected 7 principal components to retain 95.51% variance.
105 Fold 26 Training AUC: 0.9560
106 Fold 26 Test Posterior: 0.0421 (True Label: 0)
107 LOOCV Fold 27/103
108 [INFO] selected 7 principal components to retain 95.58% variance.
109 Fold 27 Training AUC: 0.9560
110 Fold 27 Test Posterior: 0.0002 (True Label: 0)
111 LOOCV Fold 28/103
112 [INFO] selected 7 principal components to retain 95.53% variance.
```

```
113 Fold 28 Training AUC: 0.9568
114 Fold 28 Test Posterior: 0.0355 (True Label: 0)
115 LOOCV Fold 29/103
116 [INFO] selected 7 principal components to retain 95.52% variance.
117 Fold 29 Training AUC: 0.9556
118 Fold 29 Test Posterior: 0.0020 (True Label: 0)
119 LOOCV Fold 30/103
120 [INFO] selected 7 principal components to retain 95.50% variance.
121 Fold 30 Training AUC: 0.9580
122 Fold 30 Test Posterior: 0.7351 (True Label: 0)
123 LOOCV Fold 31/103
124 [INFO] selected 7 principal components to retain 95.49% variance.
125 Fold 31 Training AUC: 0.9576
126 Fold 31 Test Posterior: 0.0774 (True Label: 0)
127 LOOCV Fold 32/103
128 [INFO] selected 7 principal components to retain 95.50% variance.
129 Fold 32 Training AUC: 0.9564
130 Fold 32 Test Posterior: 0.4315 (True Label: 0)
131 LOOCV Fold 33/103
132 [INFO] selected 7 principal components to retain 95.50% variance.
133 Fold 33 Training AUC: 0.9568
134 Fold 33 Test Posterior: 0.1194 (True Label: 0)
135 LOOCV Fold 34/103
136 [INFO] selected 7 principal components to retain 95.48% variance.
137 Fold 34 Training AUC: 0.9576
138 Fold 34 Test Posterior: 0.4015 (True Label: 0)
139 LOOCV Fold 35/103
140 [INFO] selected 7 principal components to retain 95.61% variance.
141 Fold 35 Training AUC: 0.9572
142 Fold 35 Test Posterior: 0.0888 (True Label: 0)
143 LOOCV Fold 36/103
144 [INFO] selected 7 principal components to retain 95.48% variance.
145 Fold 36 Training AUC: 0.9548
146 Fold 36 Test Posterior: 0.0349 (True Label: 0)
147 LOOCV Fold 37/103
148 [INFO] selected 7 principal components to retain 95.50% variance.
149 Fold 37 Training AUC: 0.9568
150 Fold 37 Test Posterior: 0.1389 (True Label: 0)
151 LOOCV Fold 38/103
152 [INFO] selected 7 principal components to retain 95.50% variance.
153 Fold 38 Training AUC: 0.9548
154 Fold 38 Test Posterior: 1.0000 (True Label: 1)
155 LOOCV Fold 39/103
156 [INFO] selected 7 principal components to retain 95.54% variance.
157 Fold 39 Training AUC: 0.9552
158 Fold 39 Test Posterior: 1.0000 (True Label: 1)
159 LOOCV Fold 40/103
160 [INFO] selected 7 principal components to retain 95.49% variance.
161 Fold 40 Training AUC: 0.9577
162 Fold 40 Test Posterior: 0.9565 (True Label: 1)
163 LOOCV Fold 41/103
164 [INFO] selected 7 principal components to retain 95.54% variance.
165 Fold 41 Training AUC: 0.9653
166 Fold 41 Test Posterior: 0.0215 (True Label: 1)
167 LOOCV Fold 42/103
168 [INFO] selected 7 principal components to retain 95.44% variance.
169 Fold 42 Training AUC: 0.9548
170 Fold 42 Test Posterior: 1.0000 (True Label: 1)
171 LOOCV Fold 43/103
```

```
172 [INFO] selected 7 principal components to retain 95.37% variance.
173 Fold 43 Training AUC: 0.9565
174 Fold 43 Test Posterior: 1.0000 (True Label: 1)
175 LOOCV Fold 44/103
176 [INFO] selected 7 principal components to retain 95.51% variance.
177 Fold 44 Training AUC: 0.9560
178 Fold 44 Test Posterior: 0.9641 (True Label: 1)
179 LOOCV Fold 45/103
180 [INFO] selected 7 principal components to retain 95.48% variance.
181 Fold 45 Training AUC: 0.9565
182 Fold 45 Test Posterior: 0.9624 (True Label: 1)
183 LOOCV Fold 46/103
184 [INFO] selected 7 principal components to retain 95.47% variance.
185 Fold 46 Training AUC: 0.9556
186 Fold 46 Test Posterior: 0.9901 (True Label: 1)
187 LOOCV Fold 47/103
188 [INFO] selected 7 principal components to retain 95.53% variance.
189 Fold 47 Training AUC: 0.9552
190 Fold 47 Test Posterior: 0.7765 (True Label: 1)
191 LOOCV Fold 48/103
192 [INFO] selected 7 principal components to retain 95.55% variance.
193 Fold 48 Training AUC: 0.9577
194 Fold 48 Test Posterior: 0.9473 (True Label: 1)
195 LOOCV Fold 49/103
196 [INFO] selected 7 principal components to retain 95.50% variance.
197 Fold 49 Training AUC: 0.9569
198 Fold 49 Test Posterior: 0.8532 (True Label: 1)
199 LOOCV Fold 50/103
200 [INFO] selected 7 principal components to retain 95.24% variance.
201 Fold 50 Training AUC: 0.9556
202 Fold 50 Test Posterior: 1.0000 (True Label: 1)
203 LOOCV Fold 51/103
204 [INFO] selected 7 principal components to retain 95.43% variance.
205 Fold 51 Training AUC: 0.9544
206 Fold 51 Test Posterior: 1.0000 (True Label: 1)
207 LOOCV Fold 52/103
208 [INFO] selected 7 principal components to retain 95.52% variance.
209 Fold 52 Training AUC: 0.9560
210 Fold 52 Test Posterior: 0.0010 (True Label: 0)
211 LOOCV Fold 53/103
212 [INFO] selected 7 principal components to retain 95.49% variance.
213 Fold 53 Training AUC: 0.9564
214 Fold 53 Test Posterior: 0.0294 (True Label: 0)
215 LOOCV Fold 54/103
216 [INFO] selected 7 principal components to retain 95.43% variance.
217 Fold 54 Training AUC: 0.9548
218 Fold 54 Test Posterior: 1.0000 (True Label: 1)
219 LOOCV Fold 55/103
220 [INFO] selected 7 principal components to retain 95.50% variance.
221 Fold 55 Training AUC: 0.9568
222 Fold 55 Test Posterior: 0.3133 (True Label: 0)
223 LOOCV Fold 56/103
224 [INFO] selected 7 principal components to retain 95.55% variance.
225 Fold 56 Training AUC: 0.9657
226 Fold 56 Test Posterior: 0.0225 (True Label: 1)
227 LOOCV Fold 57/103
228 [INFO] selected 7 principal components to retain 95.49% variance.
229 Fold 57 Training AUC: 0.9544
230 Fold 57 Test Posterior: 0.4537 (True Label: 1)
```

```
231 LOOCV Fold 58/103
232 [INFO] selected 7 principal components to retain 95.59% variance.
233 Fold 58 Training AUC: 0.9585
234 Fold 58 Test Posterior: 0.1557 (True Label: 1)
235 LOOCV Fold 59/103
236 [INFO] selected 7 principal components to retain 95.40% variance.
237 Fold 59 Training AUC: 0.9581
238 Fold 59 Test Posterior: 1.0000 (True Label: 1)
239 LOOCV Fold 60/103
240 [INFO] selected 7 principal components to retain 95.45% variance.
241 Fold 60 Training AUC: 0.9556
242 Fold 60 Test Posterior: 0.9153 (True Label: 1)
243 LOOCV Fold 61/103
244 [INFO] selected 7 principal components to retain 95.49% variance.
245 Fold 61 Training AUC: 0.9560
246 Fold 61 Test Posterior: 0.0070 (True Label: 0)
247 LOOCV Fold 62/103
248 [INFO] selected 7 principal components to retain 95.54% variance.
249 Fold 62 Training AUC: 0.9564
250 Fold 62 Test Posterior: 0.0360 (True Label: 0)
251 LOOCV Fold 63/103
252 [INFO] selected 7 principal components to retain 95.50% variance.
253 Fold 63 Training AUC: 0.9596
254 Fold 63 Test Posterior: 0.1115 (True Label: 0)
255 LOOCV Fold 64/103
256 [INFO] selected 7 principal components to retain 95.48% variance.
257 Fold 64 Training AUC: 0.9584
258 Fold 64 Test Posterior: 0.0922 (True Label: 0)
259 LOOCV Fold 65/103
260 [INFO] selected 7 principal components to retain 95.49% variance.
261 Fold 65 Training AUC: 0.9560
262 Fold 65 Test Posterior: 0.0187 (True Label: 0)
263 LOOCV Fold 66/103
264 [INFO] selected 7 principal components to retain 95.53% variance.
265 Fold 66 Training AUC: 0.9560
266 Fold 66 Test Posterior: 0.0378 (True Label: 0)
267 LOOCV Fold 67/103
268 [INFO] selected 7 principal components to retain 95.52% variance.
269 Fold 67 Training AUC: 0.9576
270 Fold 67 Test Posterior: 0.4102 (True Label: 0)
271 LOOCV Fold 68/103
272 [INFO] selected 7 principal components to retain 95.50% variance.
273 Fold 68 Training AUC: 0.9556
274 Fold 68 Test Posterior: 0.0402 (True Label: 0)
275 LOOCV Fold 69/103
276 [INFO] selected 7 principal components to retain 95.46% variance.
277 Fold 69 Training AUC: 0.9556
278 Fold 69 Test Posterior: 0.0154 (True Label: 0)
279 LOOCV Fold 70/103
280 [INFO] selected 7 principal components to retain 95.55% variance.
281 Fold 70 Training AUC: 0.9552
282 Fold 70 Test Posterior: 0.0014 (True Label: 0)
283 LOOCV Fold 71/103
284 [INFO] selected 7 principal components to retain 95.52% variance.
285 Fold 71 Training AUC: 0.9548
286 Fold 71 Test Posterior: 0.0037 (True Label: 0)
287 LOOCV Fold 72/103
288 [INFO] selected 7 principal components to retain 95.52% variance.
289 Fold 72 Training AUC: 0.9564
```

```
290 Fold 72 Test Posterior: 0.0545 (True Label: 0)
291 LOOCV Fold 73/103
292 [INFO] selected 7 principal components to retain 95.52% variance.
293 Fold 73 Training AUC: 0.9568
294 Fold 73 Test Posterior: 0.0854 (True Label: 0)
295 LOOCV Fold 74/103
296 [INFO] selected 7 principal components to retain 95.54% variance.
297 Fold 74 Training AUC: 0.9576
298 Fold 74 Test Posterior: 0.1040 (True Label: 0)
299 LOOCV Fold 75/103
300 [INFO] selected 7 principal components to retain 95.49% variance.
301 Fold 75 Training AUC: 0.9617
302 Fold 75 Test Posterior: 0.0473 (True Label: 1)
303 LOOCV Fold 76/103
304 [INFO] selected 7 principal components to retain 95.50% variance.
305 Fold 76 Training AUC: 0.9552
306 Fold 76 Test Posterior: 0.0005 (True Label: 0)
307 LOOCV Fold 77/103
308 [INFO] selected 7 principal components to retain 95.52% variance.
309 Fold 77 Training AUC: 0.9556
310 Fold 77 Test Posterior: 0.0035 (True Label: 0)
311 LOOCV Fold 78/103
312 [INFO] selected 7 principal components to retain 95.48% variance.
313 Fold 78 Training AUC: 0.9552
314 Fold 78 Test Posterior: 0.0016 (True Label: 0)
315 LOOCV Fold 79/103
316 [INFO] selected 7 principal components to retain 95.45% variance.
317 Fold 79 Training AUC: 0.9532
318 Fold 79 Test Posterior: 0.5043 (True Label: 1)
319 LOOCV Fold 80/103
320 [INFO] selected 7 principal components to retain 95.48% variance.
321 Fold 80 Training AUC: 0.9573
322 Fold 80 Test Posterior: 1.0000 (True Label: 1)
323 LOOCV Fold 81/103
324 [INFO] selected 7 principal components to retain 95.51% variance.
325 Fold 81 Training AUC: 0.9556
326 Fold 81 Test Posterior: 0.0146 (True Label: 0)
327 LOOCV Fold 82/103
328 [INFO] selected 7 principal components to retain 95.48% variance.
329 Fold 82 Training AUC: 0.9556
330 Fold 82 Test Posterior: 0.0054 (True Label: 0)
331 LOOCV Fold 83/103
332 [INFO] selected 7 principal components to retain 95.48% variance.
333 Fold 83 Training AUC: 0.9548
334 Fold 83 Test Posterior: 0.9959 (True Label: 1)
335 LOOCV Fold 84/103
336 [INFO] selected 7 principal components to retain 95.46% variance.
337 Fold 84 Training AUC: 0.9536
338 Fold 84 Test Posterior: 1.0000 (True Label: 1)
339 LOOCV Fold 85/103
340 [INFO] selected 7 principal components to retain 95.50% variance.
341 Fold 85 Training AUC: 0.9552
342 Fold 85 Test Posterior: 1.0000 (True Label: 1)
343 LOOCV Fold 86/103
344 [INFO] selected 7 principal components to retain 95.48% variance.
345 Fold 86 Training AUC: 0.9540
346 Fold 86 Test Posterior: 0.7460 (True Label: 1)
347 LOOCV Fold 87/103
348 [INFO] selected 7 principal components to retain 95.54% variance.
```

```
349 Fold 87 Training AUC: 0.9552
350 Fold 87 Test Posterior: 0.9895 (True Label: 1)
351 LOOCV Fold 88/103
352 [INFO] selected 7 principal components to retain 95.50% variance.
353 Fold 88 Training AUC: 0.9548
354 Fold 88 Test Posterior: 0.9999 (True Label: 1)
355 LOOCV Fold 89/103
356 [INFO] selected 7 principal components to retain 95.48% variance.
357 Fold 89 Training AUC: 0.9564
358 Fold 89 Test Posterior: 0.0167 (True Label: 0)
359 LOOCV Fold 90/103
360 [INFO] selected 7 principal components to retain 95.52% variance.
361 Fold 90 Training AUC: 0.9608
362 Fold 90 Test Posterior: 0.8152 (True Label: 0)
363 LOOCV Fold 91/103
364 [INFO] selected 7 principal components to retain 95.49% variance.
365 Fold 91 Training AUC: 0.9564
366 Fold 91 Test Posterior: 0.0020 (True Label: 0)
367 LOOCV Fold 92/103
368 [INFO] selected 7 principal components to retain 95.49% variance.
369 Fold 92 Training AUC: 0.9544
370 Fold 92 Test Posterior: 0.9862 (True Label: 1)
371 LOOCV Fold 93/103
372 [INFO] selected 7 principal components to retain 95.44% variance.
373 Fold 93 Training AUC: 0.9565
374 Fold 93 Test Posterior: 1.0000 (True Label: 1)
375 LOOCV Fold 94/103
376 [INFO] selected 7 principal components to retain 95.40% variance.
377 Fold 94 Training AUC: 0.9565
378 Fold 94 Test Posterior: 1.0000 (True Label: 1)
379 LOOCV Fold 95/103
380 [INFO] selected 7 principal components to retain 95.41% variance.
381 Fold 95 Training AUC: 0.9585
382 Fold 95 Test Posterior: 1.0000 (True Label: 1)
383 LOOCV Fold 96/103
384 [INFO] selected 7 principal components to retain 95.50% variance.
385 Fold 96 Training AUC: 0.9532
386 Fold 96 Test Posterior: 0.7928 (True Label: 1)
387 LOOCV Fold 97/103
388 [INFO] selected 7 principal components to retain 95.60% variance.
389 Fold 97 Training AUC: 0.9577
390 Fold 97 Test Posterior: 0.8888 (True Label: 1)
391 LOOCV Fold 98/103
392 [INFO] selected 7 principal components to retain 95.50% variance.
393 Fold 98 Training AUC: 0.9585
394 Fold 98 Test Posterior: 0.9953 (True Label: 1)
395 LOOCV Fold 99/103
396 [INFO] selected 7 principal components to retain 95.47% variance.
397 Fold 99 Training AUC: 0.9528
398 Fold 99 Test Posterior: 0.9996 (True Label: 1)
399 LOOCV Fold 100/103
400 [INFO] selected 7 principal components to retain 95.53% variance.
401 Fold 100 Training AUC: 0.9565
402 Fold 100 Test Posterior: 0.9940 (True Label: 1)
403 LOOCV Fold 101/103
404 [INFO] selected 7 principal components to retain 95.48% variance.
405 Fold 101 Training AUC: 0.9581
406 Fold 101 Test Posterior: 1.0000 (True Label: 1)
407 LOOCV Fold 102/103
```

```

408 [INFO] selected 7 principal components to retain 95.53% variance.
409 Fold 102 Training AUC: 0.9548
410 Fold 102 Test Posterior: 0.9295 (True Label: 1)
411 LOOCV Fold 103/103
412 [INFO] selected 7 principal components to retain 95.51% variance.
413 Fold 103 Training AUC: 0.9746
414 Fold 103 Test Posterior: 0.0020 (True Label: 1)
415
416 [INFO] LOOCV Finished

```

B Eigenvalues and their eigenvectors

```

1 [1] Eigenvalue = 9.254088
2     Eigenvector = [-0.24610304 -0.25236568 -0.23797428 -0.25584874 -0.27877536 -0.2474438
3 -0.16716238 -0.28522706 -0.25914694 -0.16994276 -0.20843513 -0.13799287
4 -0.21603919 -0.13923098 -0.21570834 -0.27832607 -0.27492191 -0.25586974
5 -0.12562907]
6
7 [2] Eigenvalue = 3.874613
8     Eigenvector = [-0.26725741 -0.25407227 -0.25785828 -0.25825467 -0.0021897  0.1156356
9 0.15676828 0.01352183 0.13683749 -0.21376507 0.36563198 0.32754076
10 0.31808514 0.32727949 0.30155406 -0.13934574 -0.16451395 -0.1384262
11 0.14980121]
12
13 [3] Eigenvalue = 1.869370
14     Eigenvector = [ 0.11882603 0.17056818 0.19766062 0.10992857 -0.29297118 -0.35329359
15 -0.29584155 -0.26193397 -0.30841329 -0.01634261 0.15491728 0.36115102
16 -0.02145898 0.349847 -0.05720395 0.05792253 0.05568495 0.14443001
17 0.36823352]
18
19 [4] Eigenvalue = 1.058813
20     Eigenvector = [ 0.1807304 0.18418271 0.1118217 0.18543043 0.16486044 0.20384531
21 -0.11000757 0.16560143 0.2056896 -0.43489067 -0.06579517 0.27809191
22 -0.29369659 0.27899271 -0.32975119 -0.16722578 -0.17377102 -0.33697645
23 -0.14359909]
24
25 [5] Eigenvalue = 0.904257
26     Eigenvector = [ 0.27036456 0.18892724 0.18873248 0.23188112 -0.25368368 -0.14873459
27 0.54407781 -0.23367672 -0.13110369 -0.0777008 0.12192098 -0.01396198
28 0.19215762 -0.0392042 0.19178693 -0.19177759 -0.23080416 -0.08981169
29 -0.39124607]
30
31 [6] Eigenvalue = 0.687637
32     Eigenvector = [-0.0316842 -0.10206292 -0.08173363 -0.05370322 0.03846078 0.0497094
33 -0.21042741 -0.00973693 -0.01205271 0.56097967 0.08913477 0.28076712
34 -0.06349212 0.28822653 -0.08408869 -0.11279121 -0.0596503 0.19252034
35 -0.61769787]
36
37 [7] Eigenvalue = 0.494327
38     Eigenvector = [-0.02033025 -0.15958501 -0.2698188 -0.02994783 0.05715444 -0.2752525
39 0.33202595 0.09380796 -0.2146118 -0.28544235 -0.02518313 0.13568201
40 -0.13290314 0.16003251 -0.1391034 0.47286466 0.43321256 -0.0023878
41 -0.28612226]
42
43 [8] Eigenvalue = 0.330288

```

```
44     Eigenvector = [-0.03217798 -0.03893844 -0.02878806 -0.06398944 -0.13550947 -0.00887977
45     0.57078621  0.00769898  0.16723256  0.46623072 -0.12488319  0.14381288
46     -0.28904055  0.11695917 -0.3161676  -0.042398  -0.06543884 -0.14235019
47     0.37826197]
48
49 [9] Eigenvalue = 0.187203
50     Eigenvector = [ 0.13461388  0.05743389 -0.15767414  0.15941761  0.08784267 -0.24537752
51     -0.19563238  0.18830587 -0.10772536  0.33118423  0.10764955 -0.00845869
52     0.16798453 -0.06145598  0.13635586  0.07701927  0.10359309 -0.76530591
53     0.02747448]
54
55 [10] Eigenvalue = 0.118827
56     Eigenvector = [ 0.44206499 -0.19901913 -0.61223485  0.36161105 -0.20589131 -0.12910798
57     -0.09549129  0.07996993  0.28558134 -0.03986784  0.00549191  0.00287252
58     0.00656165 -0.07774238 -0.020817  -0.06417484 -0.13350493  0.25236131
59     0.09730849]
60
61 [11] Eigenvalue = 0.080670
62     Eigenvector = [ 0.22723751 -0.11259803 -0.19512359  0.09496643  0.10729184  0.62134116
63     -0.0007445  -0.56172936 -0.29488158  0.05210895  0.02545448  0.04883718
64     0.00451878 -0.03252664 -0.05659866  0.22784088  0.02508112 -0.14388207
65     0.07244501]
66
67 [12] Eigenvalue = 0.054409
68     Eigenvector = [ 3.26297804e-02 -1.53911519e-01  2.44292223e-01 -1.23569771e-01
69     -5.49992498e-01  8.11758888e-02 -1.53046801e-01 -1.81083034e-01
70     5.47549027e-01 -1.83687108e-02  1.20819398e-03 -6.07026455e-02
71     4.69034045e-02  3.57683204e-02  2.93713772e-04  3.80825560e-01
72     1.26989569e-01 -2.03359448e-01 -1.58682613e-01]
73
74 [13] Eigenvalue = 0.032970
75     Eigenvector = [ 0.09384293 -0.04974429 -0.03309492  0.02997972  0.03640106  0.00634576
76     0.00660325 -0.00634433 -0.0526088  0.02967933 -0.30812593 -0.53605875
77     -0.08519016  0.70423744  0.29401083  0.02271996 -0.08395705 -0.02295224
78     0.03980924]
79
80 [14] Eigenvalue = 0.018747
81     Eigenvector = [-0.13550287  0.36012575 -0.2275393  -0.01047853 -0.09555848  0.06280675
82     0.01082823 -0.09095079  0.06957397 -0.00918721  0.14801668 -0.30866373
83     0.44674542  0.19188292 -0.52965502 -0.21945337  0.30124816  0.00820919
84     -0.02406894]
85
86 [15] Eigenvalue = 0.016615
87     Eigenvector = [-0.24850113  0.57494247 -0.34977836  0.01048763 -0.16958541  0.09581791
88     -0.01290136 -0.14837106  0.13080026  0.00230297 -0.14742897  0.15353393
89     -0.33528812 -0.0596299  0.42538848 -0.08659168  0.23524241 -0.021232
90     -0.04973586]
91
92 [16] Eigenvalue = 0.012510
93     Eigenvector = [-0.17499955  0.38144775 -0.1738592  -0.05105404  0.02173639 -0.04762936
94     -0.01735169  0.06929979 -0.02024213  0.03179349  0.04244829 -0.04229477
95     0.09832144  0.00133841 -0.12899108  0.57609997 -0.64531711  0.05350596
96     -0.02622141]
97
98 [17] Eigenvalue = 0.004353
99     Eigenvector = [-0.59958719 -0.21942205  0.07975273  0.75855322 -0.05230213  0.04555105
100     0.00742571 -0.0414711  0.00451455  0.01073608 -0.00081973 -0.01870468
101     0.00490655  0.02972955 -0.02297988  0.04065851 -0.01603002 -0.01255848
102     -0.00321064]
```

```
103
104 [18] Eigenvalue = 0.000299
105     Eigenvector = [ 1.93810567e-02  4.32028274e-04 -1.12145861e-02 -1.14975488e-02
106 -5.61471995e-01  4.14175594e-01 -4.44566100e-03  5.76037050e-01
107 -4.24553052e-01 -4.59354706e-03  6.12855028e-03  1.80605162e-04
108 -6.08677052e-03 -1.31521277e-03  4.38701293e-03 -1.37153660e-02
109  1.14527296e-02  7.35555682e-03  4.07669801e-04]
110
111 [19] Eigenvalue = 0.000005
112     Eigenvector = [-2.12051475e-03 -1.14640840e-03  3.39339262e-04  2.81025647e-03
113 -4.36238799e-03  3.26440886e-03  5.36196604e-04  4.25716628e-03
114 -3.75581770e-03  5.59046768e-05 -7.76405862e-01  3.65102177e-01
115  5.13614502e-01 -1.03489742e-03  3.75756778e-03 -1.53407944e-03
116  8.96618401e-04  1.93197429e-04  2.56301617e-04]
```
