

MTH 602 Scientific Machine Learning

Homework 4

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I. PAPER & PENCIL WORK

1. (i) A positive definite matrix of the size $D \times D$ is symmetric, and can be written in the form:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & \dots & a_{1D} \\ a_{12} & a_{22} & a_{23} & \dots & \dots & a_{2D} \\ a_{13} & a_{23} & a_{33} & \dots & \dots & a_{3D} \\ \vdots & \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & \vdots & & \ddots & \vdots \\ a_{1D} & a_{2D} & a_{3D} & \dots & \dots & a_{DD} \end{bmatrix}$$

The no. of diagonal elements in A are D and the no. of off-diagonal elements are $(D^2 - D)$, but since this is a symmetric matrix, only half of them will be independent. As a result, the no. of the independent off-diagonal elements will be $(D^2 - D)/2$. So, the total no. of independent parameters is

$$D + \frac{D^2 - D}{2} = \frac{D(D+1)}{2} \quad (\text{Ans.})$$

- (ii) The no. of independent parameters in a D -dimensional Gaussian should be the sum of total parameters in symmetric $D \times D$ co-variance matrix, Σ and D -dimensional mean vector, μ .

No. of independent parameters in $\Sigma = D(D+1)/2$ [as obtained from (i)].

No. of independent parameters in $\mu = D$ [since, its dimension is D].

So, total no. of independent parameters in a D -dimensional Gaussian is

$$\frac{D(D+1)}{2} + D = \frac{D(D+3)}{2} \quad (\text{Ans.})$$

- (iii) Gaussian mixture model (GMM) can be written as,

$$p(\mathbf{x}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x} | \mu_k, \Sigma_k)$$

where, π_k are mixing coefficients and $\sum_{k=1}^K \pi_k = 1$.

Since, each D -dimensional Gaussian has $\frac{D(D+3)}{2}$ independent parameters, GMM with K components will have total independent parameters as a summation of the independent parameters due to GMM and the mixing coefficients. Since, the total K mixing coefficients sums up to 1, the no. of independent coefficients will be the degree of freedom, which is $(K-1)$. So, the total no. of independent parameters are

$$K \frac{D(D+3)}{2} + (K-1) \quad (\text{Ans.})$$

II. CHAPTER 3: MULTIVARIATE GAUSSIAN MIXTURE MODELING

A. Stage 1 — One Gaussian: MLE vs. GMM with 1 component

Given ground-truth Gaussian:

$$\mu = (2, -1), \quad \Sigma = \begin{bmatrix} 2 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$

1. Computed eigen-values:

$$\lambda_1 = 2.44339811320566, \quad \lambda_2 = 0.5566018867943396$$

Computed eigen-vectors:

$$\mathbf{u}_1 = \begin{pmatrix} -0.8746424812468178 \\ -0.4847685323929453 \end{pmatrix}, \quad \mathbf{u}_2 = \begin{pmatrix} 0.4847685323929453 \\ -0.8746424812468178 \end{pmatrix}$$

Principal axes and orientation of ellipse:

$$2\lambda_1^{\frac{1}{2}} = 3.1262745325423102, \quad 2\lambda_2^{\frac{1}{2}} = 1.492115125309491, \quad \theta = 28.997308395958242^\circ$$

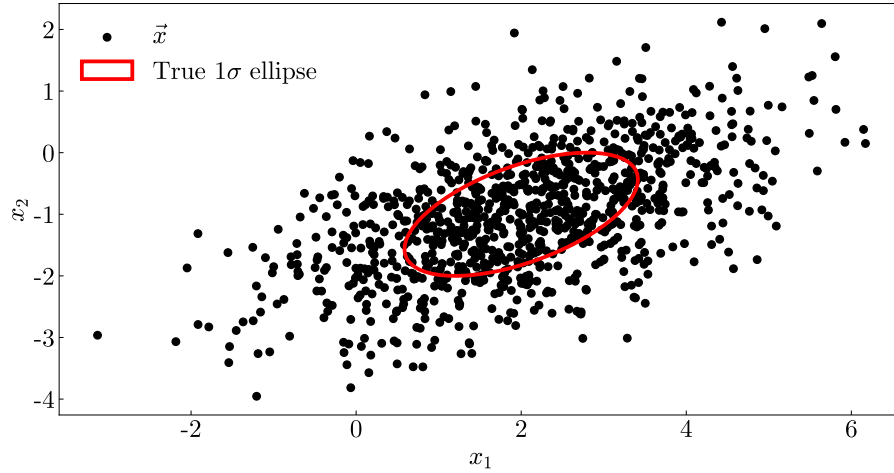


Figure 1: 1000 samples $\vec{x} \sim \mathcal{N}(\mu, \Sigma)$ drawn using `sample_2d_gaussian` along with true 1σ ellipse of Σ .

2. Analytic maximum likelihood solution:

$$\hat{\mu} = (2.014655285377038, -1.0132083392419486),$$

$$\hat{\Sigma} = \begin{bmatrix} 2.069533458212539 & 0.7855473289101127 \\ 0.7855473289101127 & 0.9810586095342764 \end{bmatrix}$$

Percentage relative error compared to ground-truth solution:

$$\delta\mu = \frac{|\hat{\mu}_i - \mu_i|}{|\mu_i|} \times 100\% = (0.7327642688518932\%, 1.3208339241948641\%),$$

$$\hat{\Sigma} = \frac{|\hat{\Sigma}_{ij} - \Sigma_{ij}|}{|\Sigma_{ij}|} \times 100\% = \begin{bmatrix} 3.4766729106269434\% & 1.8065838862359185\% \\ 1.8065838862359185\% & 1.8941390465723629\% \end{bmatrix}$$

The analytic maximum likelihood solution is close to the ground truth solution within a comparatively small upper error bound of $\sim 1.5\%$ for mean and $\sim 3.5\%$ for co-variance.

3. Fitted one-component GMM:

$$\mu_{gmm} = (2.014655285377037, -1.0132083392419482),$$

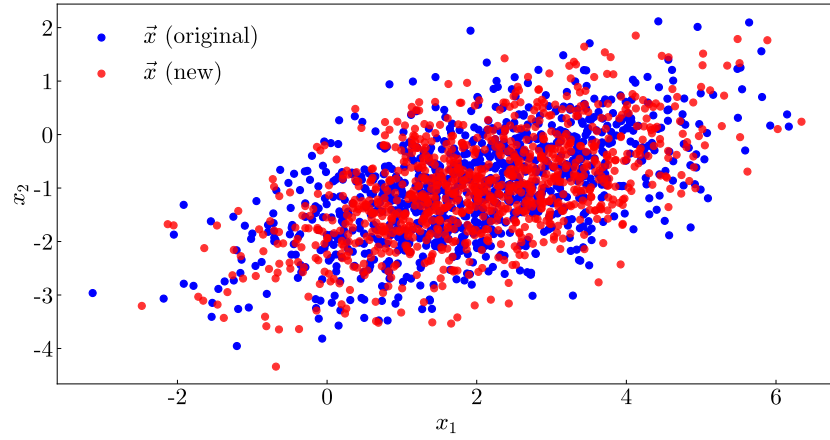
$$\Sigma_{gmm} = \begin{bmatrix} 2.0695344582125386 & 0.7855473289101127 \\ 0.7855473289101127 & 0.9810596095342764 \end{bmatrix}$$

Comparison to the maximum likelihood solution:

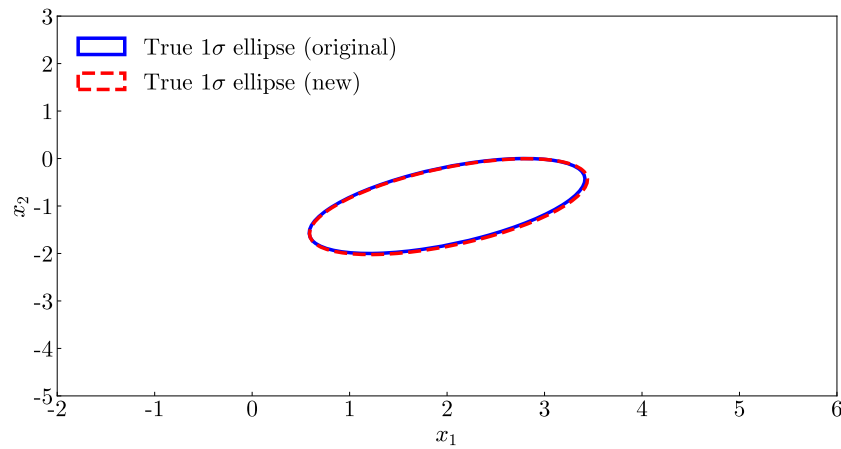
$$\|\hat{\mu} - \mu_{gmm}\|_2 = 9.930136612989092 \times 10^{-16}, \quad \|\hat{\Sigma} - \Sigma_{gmm}\|_2 = 1.0000000000287557 \times 10^{-06}$$

Agreement is very close.

4. New points ($M = 1000$) are drawn from the fitted one-component GMM model.



(a)



(b)

Figure 2: (a) Overlay of new samples on the original samples. (b) True 1σ ellipse of Σ for new and original samples.

B. Stage 2 — Two-component mixture in 2D: Fit, Compare, Sample, Classify

Given ground truth mixture:

$$\omega = (0.2, 0.8); \quad \mu_1 = (0, 0), \quad \Sigma_1 = \begin{bmatrix} 1 & 0.6 \\ 0.6 & 1.5 \end{bmatrix}; \quad \mu_2 = (4, 3), \quad \Sigma_2 = \begin{bmatrix} 1.2 & -0.5 \\ -0.5 & 0.8 \end{bmatrix}$$

Observed pulsar population:

$$P(\vec{x}) = 0.2\mathcal{N}(\vec{x}|\mu_1, \Sigma_1) + 0.8\mathcal{N}(\vec{x}|\mu_2, \Sigma_2)$$

1. Sampling of the two components and their corresponding Gaussian $\vec{x} \sim \mathcal{N}(\mu_1, \Sigma_1)$ and $\vec{x} \sim \mathcal{N}(\mu_2, \Sigma_2)$ respectively:

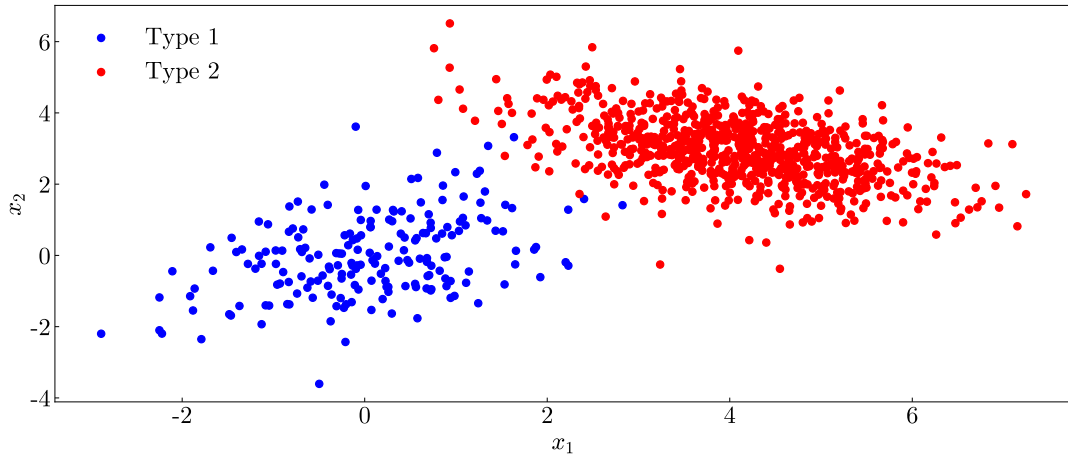


Figure 3: Total 1000 samples drawn from $\vec{x} \sim \mathcal{N}(\mu_1, \Sigma_1)$ and $\vec{x} \sim \mathcal{N}(\mu_2, \Sigma_2)$ for type-1 and type-2 pulsar using `sample_2d_gaussian`.

2. Fitted GMM for $K = 1$:

$$\mu_{gmm} = (3.3043244939443674, 2.3696992901480693),$$

$$\Sigma_{gmm} = \begin{bmatrix} 3.6926089015268726 & 1.561316587647234 \\ 1.561316587647234 & 2.25828069278701 \end{bmatrix}$$

Fitted GMM for $K = 2$:

$$\mu_{1,gmm} = (0.0887631709875105, -0.0210976144553744),$$

$$\Sigma_{1,gmm} = \begin{bmatrix} 1.0761406229476318 & 0.476672845843364 \\ 0.476672845843364 & 1.229744902269525 \end{bmatrix};$$

$$\mu_{2,gmm} = (4.0816341486534675, 2.9476355599773143),$$

$$\Sigma_{2,gmm} = \begin{bmatrix} 1.2214003949426913 & -0.4841133862236404 \\ -0.4841133862236405 & 0.7911739159757286 \end{bmatrix}$$

It is easily evident that $K = 2$ produces the means and co-variances that are closer to the ground truth means and co-variances.

Diagnostics for these two models are compared using log-likelihood and Bayesian information criterion diagnostics:

$$\text{log-likelihood}_{K=1} : -3725.457633, \quad \text{log-likelihood}_{K=2} : -3200.461304$$

$$\text{Bayesian information criterion}_{K=1} : 7485.454043,$$

$$\text{Bayesian information criterion}_{K=2} : 6476.907916$$

Higher value for the log-likelihood and lower value for Bayesian information criterion are desired for the preferred model. Since, log-likelihood is greater for $K = 2$ than $K = 1$ and Bayesian information criterion is smaller for $K = 2$ than $K = 1$, GMM for $K = 2$ is the better and preferred model.

3. For $K = 2$,

Weights:

$$\omega_1 = 0.1946743731658157, \quad \omega_2 = 0.8053256268341843$$

Means:

$$\hat{\mu}_1 = (0.0887631709875105, -0.0210976144553744),$$

$$\hat{\mu}_2 = (4.0816341486534675, 2.9476355599773143)$$

Predicted $\hat{\mu}_k$ is close to true μ_k . The maximum deviation is $\sim \pm 0.09$.

Co-variances:

$$\hat{\Sigma}_1 = \begin{bmatrix} 1.0761406229476318 & 0.476672845843364 \\ 0.476672845843364 & 1.229744902269525 \end{bmatrix};$$

$$\hat{\Sigma}_2 = \begin{bmatrix} 1.2214003949426913 & -0.4841133862236404 \\ -0.4841133862236405 & 0.7911739159757286 \end{bmatrix}$$

Predicted $\hat{\Sigma}_2$ gives very good estimation to true Σ_2 while Predicted $\hat{\Sigma}_1$ is a bit off compared to true Σ_1 , which can be attributed to the small sample size for that component.

4. New sampled data cover type-2 mode really well compared to the true sampled data as can

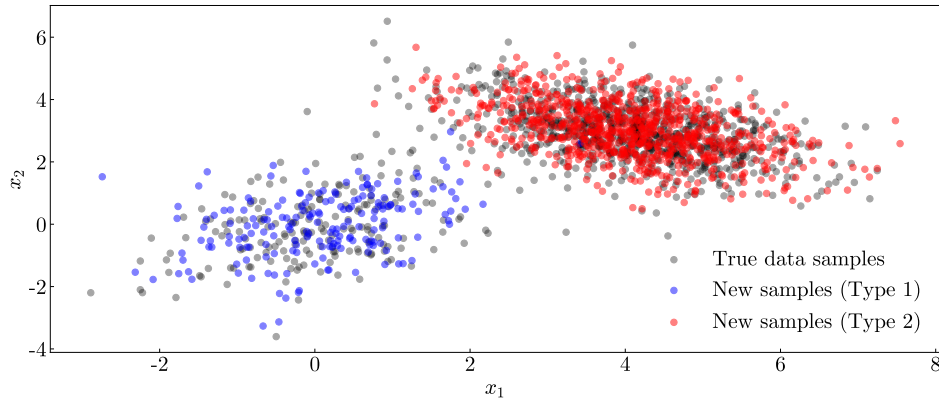


Figure 4: Samples drawn from fitted GMM.

be seen from figure 4. Type-1 mode is also covered well but it is not covered as good as type-2. However, the overlap between the two modes is minimal which is a good sign for classification.

5. Classifier's accuracy = $0.998 = 99.8\%$

	Predicted: Type-1	Predicted: Type-2
Actual: Type-1	184	1
Actual: Type-2	1	814

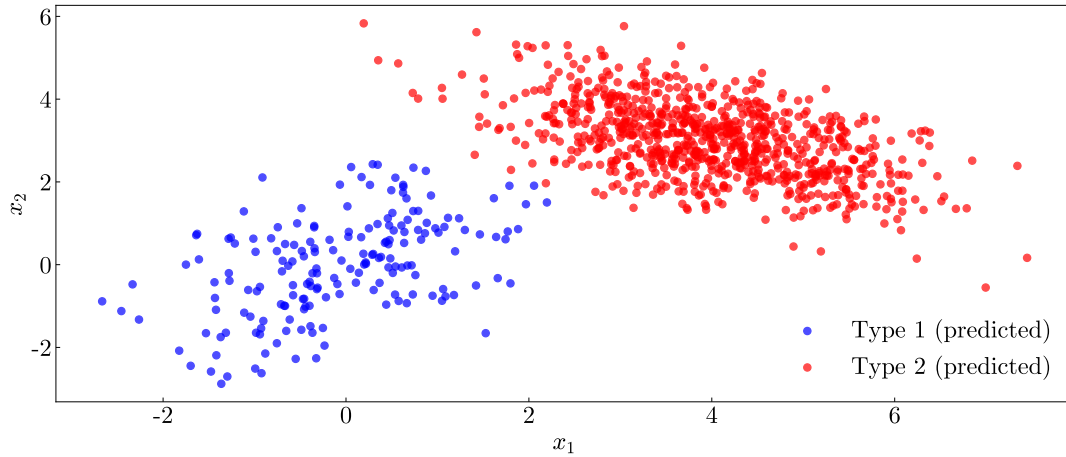


Figure 5: Visual check for classification of pulsar type.

The two-component GMM classifier is working really good with only two misclassifications out of 1000 data samples. It falsely classifies only one type-1 out of 185 samples, and one type-2 as type-1 out of 815 samples, which is a great prediction accuracy.

```

1 from sklearn.mixture import GaussianMixture
2 from sklearn.metrics import confusion_matrix, accuracy_score
3 from scipy.special import logsumexp
4 import numpy as np
5 import matplotlib.pyplot as plt
6 import matplotlib as mpl
7 from matplotlib.patches import Ellipse
8
9 # ===== II. CHAPTER 3: MULTIVARIATE GAUSSIAN MIXTURE MODELING =====
10 def sample_2d_gaussian(mu, Sigma, n, rng=None):
11     if rng is None:
12         rng = np.random.default_rng()
13     return rng.multivariate_normal(mean=mu, cov=Sigma, size=n)
14
15 # ===== A. STAGE 1: ONE GAUSSIAN: MLE VS. GMM WITH 1 COMPONENT =====
16 mu = np.array([2, -1])
17 Sigma = np.array([[2, 0.8], [0.8, 1]])
18 rng = np.random.default_rng(29)
19 n = 1000
20
21 # ===== 1. Visualization =====
22 # sampling
23 x = sample_2d_gaussian(mu, Sigma, n, rng)
24
25 np.set_printoptions(precision=16, suppress=False)

```

```

26 print("1.")
27 print("x: ", x)
28
29 # compute eigenvalues and eigenvectors, and sort them
30 eigen_val, eigen_vec = np.linalg.eigh(Sigma)
31 order = np.argsort(eigen_val)[::-1] # descending order
32 eigen_val = eigen_val[order]
33 eigen_vec = eigen_vec[:, order]
34
35 print("\nEigen values: ", eigen_val)
36 print("\nEigen vectors: ", eigen_vec)
37
38 #  $\Sigma$  ellipse parameters
39 wid = 2*np.sqrt(eigen_val[0]) # major axis
40 hei = 2*np.sqrt(eigen_val[1]) # minor axis
41 angle = np.degrees(np.arctan2(eigen_vec[1,0], eigen_vec[0,0])) % 180 #
    orientation
42
43 print("\nWidth: ", wid)
44 print("\nHeight: ", hei)
45 print(f"\nAngle: {angle} degree")
46
47 # parameters for plotting
48 plt.rcParams["font.family"] = "serif"
49 plt.rcParams["font.serif"] = ["CMU Serif"]
50 plt.rcParams["mathtext.fontset"] = "cm"
51 plt.rcParams["font.size"] = 20
52 mpl.rcParams["axes.unicode_minus"] = False
53
54 # scatter plot (with  $\Sigma$  of  $\Sigma$ )
55 fig, ax = plt.subplots(figsize=(12, 6))
56 ax.scatter(x[:,0], x[:,1], color="black", label=r"$\vec{x}$")
57 ax.add_patch(Ellipse(mu, wid, hei, angle=angle, edgecolor='r', fill=False, lw
    =3, label=r"True  $\Sigma$  ellipse"))
58 plt.xlabel(r"$x_1$")
59 plt.ylabel(r"$x_2$")
60 plt.legend(loc="upper left", frameon=False)
61 plt.tick_params(axis="both", which="both", direction="in")
62 plt.savefig(f"x_sample.pdf", dpi=1080)
63 plt.show()
64
65 # ===== 2. Analytic maximum-likelihood solution =====
66 mu_hat = x.mean(axis=0)
67 Sigma_hat = ((x - mu_hat).T @ (x - mu_hat)) / len(x)
68 print("\n2.")
69 print(f"Maximum likelihood: mu_hat = ", mu_hat)
70 print(f"Maximum likelihood: Sigma_hat = ", Sigma_hat)
71
72 # ===== 3. GMM with one component =====
73 g1 = GaussianMixture(n_components=1, covariance_type='full', n_init=10,
    random_state=0).fit(x) # one-component fit
74 mu_gmm = g1.means_[0] # mean
75 Sigma_gmm = g1.covariances_[0] # covariance
76 print("\n3.")
77 print(f"GMM w/ one component: mu_gmm = ", mu_gmm)
78 print(f"GMM w/ one component: Sigma_gmm = ", Sigma_gmm)
79
80 mu_err = np.linalg.norm(mu_hat - mu_gmm) # L2 norm
81 Sigma_err = np.linalg.norm(Sigma_hat - Sigma_gmm, 2) # matrix 2-norm

```



```

82 print(f"\nmu_error:", mu_err)
83 print(f"\nSigma_error:", Sigma_err)
84
85 # ===== 4. Sampling from the fitted model =====
86 m = 1000
87 x_new, _ = g1.sample(m)
88
89 print("\n4.")
90 print("x (new): ", x_new)
91
92 # compute eigenvalues and eigenvectors, and sort them
93 eigen_val_new, eigen_vec_new = np.linalg.eigh(Sigma_gmm)
94 order_new = np.argsort(eigen_val_new)[::-1]
95 eigen_val_new = eigen_val_new[order_new]
96 eigen_vec_new = eigen_vec_new[:, order_new]
97
98 print("\nEigen values (new): ", eigen_val_new)
99 print("\nEigen vectors (new): ", eigen_vec_new)
100
101 # $1\sigma$ ellipse parameters
102 wid_new = 2 * np.sqrt(eigen_val_new[0])
103 hei_new = 2 * np.sqrt(eigen_val_new[1])
104 angle_new = np.degrees(np.arctan2(eigen_vec_new[1,0], eigen_vec_new[0,0])) %
    180
105
106 print("\nWidth (new): ", wid_new)
107 print("\nHeight (new): ", hei_new)
108 print(f"\nAngle (new): {angle_new} degree")
109
110 # scatter plot (with $1\sigma$ of $\Sigma$)
111 fig, ax = plt.subplots(figsize=(12, 6))
112 ax.scatter(x[:,0], x[:,1], color="blue", label=r"$\vec{x}$ (original)")
113 ax.scatter(x_new[:,0], x_new[:,1], color="red", alpha=0.8, label=r"$\vec{x}$ (
    new)")
114 plt.xlabel(r"$x_1$")
115 plt.ylabel(r"$x_2$")
116 plt.legend(loc="upper left", frameon=False)
117 plt.tick_params(axis="both", which="both", direction="in")
118 plt.savefig(f"x_valid1.pdf", dpi=1080)
119 plt.show()
120
121 # ellipses
122 fig, ax = plt.subplots(figsize=(12, 6))
123 ax.add_patch(Ellipse(mu, wid, hei, angle=angle, edgecolor="blue", fill=False,
    lw=3, label=r"True 1$\sigma$ ellipse (original)"))
124 ax.add_patch(Ellipse(mu_gmm, wid_new, hei_new, linestyle="--", angle=angle,
    edgecolor="red", fill=False, lw=3, label=r"True 1$\sigma$ ellipse (new)"))
125 ax.set_xlim(mu[0] - 4, mu[0] + 4)
126 ax.set_ylim(mu[1] - 4, mu[1] + 4)
127 plt.xlabel(r"$x_1$")
128 plt.ylabel(r"$x_2$")
129 plt.legend(loc="upper left", frameon=False)
130 plt.tick_params(axis="both", which="both", direction="in")
131 plt.savefig(f"x_valid2.pdf", dpi=1080)
132 plt.show()
133
134 # ===== STAGE 2: TWO-COMPONENT MIXTURE IN 2D: FIT, COMPARE, SAMPLE, CLASSIFY
    =====
135 w_true = np.array([0.2, 0.8])

```

```

136 mu1 = np.array([0.0, 0.0])
137 Sigma1 = np.array([[1.0, 0.6], [0.6, 1.5]])
138 mu2 = np.array([4.0, 3.0])
139 Sigma2 = np.array([[1.2, -0.5], [-0.5, 0.8]])
140
141 z = rng.choice([0, 1], size=n, p=[0.2, 0.8])
142 x_ = np.zeros((n, 2))
143
144 # ===== 1. Visualization =====
145 # sampling
146 for k in [0, 1]:
147     n_ = np.sum(z==k)
148     x_[z==k] = sample_2d_gaussian([mu1, mu2][k], [Sigma1, Sigma2][k], n_, rng)
149
150 # scatter plot
151 fig, ax = plt.subplots(figsize=(15, 6))
152
153 ax.scatter(x_[z==0, 0], x_[z==0, 1], color='blue', label='Type 1')
154 ax.scatter(x_[z==1, 0], x_[z == 1, 1], c='red', label='Type 2')
155
156 plt.xlabel(r'$x_1$')
157 plt.ylabel(r'$x_2$')
158 plt.legend(loc="upper left", frameon=False)
159 plt.tick_params(axis="both", which="both", direction="in")
160 plt.savefig(f'x_sample2.pdf', dpi=1080)
161 plt.show()
162
163 # ===== 2. Modeling =====
164 # fit GMMs
165 g1 = GaussianMixture(n_components=1, covariance_type='full', random_state=42)
166 g1.fit(x_)
167 print("\n2. ")
168 print("For K=1,\nMean:", g1.means_)
169 print("\nCovariance:", g1.covariances_)
170
171 g2 = GaussianMixture(n_components=2, covariance_type='full', random_state=42)
172 g2.fit(x_)
173 print("\nFor K=2,\nMean:", g2.means_)
174 print("\nCovariance:", g2.covariances_)
175
176 # compute diagnostics
177 logL1, bic1 = g1.score(x_) * len(x_), g1.bic(x_)
178 logL2, bic2 = g2.score(x_) * len(x_), g2.bic(x_)
179
180 print(f"\nK=1: log-likelihood = {logL1:.16f}, Bayesian information criterion =
181       {bic1:.16f}")
182
183 print(f"\nK=2: log-likelihood = {logL2:.16f}, Bayesian information criterion =
184       {bic2:.16f}")
185
186 # ===== 3. Comparisons =====
187 means2, covs2, weights2 = g2.means_, g2.covariances_, g2.weights_
188 print("\n3. ")
189 print("For K = 2, ")
190 print(f"\nWeights: ", weights2)
191 print(f"\nMeans: ", means2)
192 print(f"\nCovariances: ", covs2)
193
194 # ===== Sampling from the fitted model =====
195 x1_new, z_new = g2.sample(m)

```

```

193
194 # scatter plot
195 fig, ax = plt.subplots(figsize=(15, 6))
196 ax.scatter(x_[:,0], x_[:,1], color="black", alpha=0.35, label="True data
    samples")
197 ax.scatter(x1_new[z_new==0, 0], x1_new[z_new==0, 1], color="blue", alpha=0.5,
    label="New samples (Type 1)")
198 ax.scatter(x1_new[z_new==1, 0], x1_new[z_new==1, 1], c="red", alpha=0.5, label
    ="New samples (Type 2)")
199
200 plt.xlabel(r"$x_1$")
201 plt.ylabel(r"$x_2$")
202 plt.legend(loc="lower right", frameon=False)
203 plt.tick_params(axis="both", which="both", direction="in")
204 plt.savefig(f"x_sample_from_fit.pdf", dpi=1080)
205 plt.show()
206
207 # ===== 5. Classification =====
208 # setup
209 n_test = 1000
210 rng = np.random.default_rng(129)
211 z_true = rng.choice([0, 1], size=n_test, p=w_true)
212 x_test = np.zeros((n_test, 2))
213
214 # constructing ground truth by sampling and testing the GMM model
215 for k in [0, 1]:
216     n_ = np.sum(z_true==k)
217     x_test[z_true==k] = sample_2d_gaussian([mu1, mu2][k], [Sigma1, Sigma2][k],
        n_, rng)
218
219 predicted_labels = g2.predict(x_test)
220
221 print("\n5. ")
222 #print(f"Predicted labels: ", predicted_labels)
223
224 # plots
225 fig, ax = plt.subplots(figsize=(15, 6))
226 ax.scatter(x_test[predicted_labels==0,0], x_test[predicted_labels==0,1], color
    ="blue",
227             alpha=0.7, label="Type 1 (predicted)")
228 ax.scatter(x_test[predicted_labels==1,0], x_test[predicted_labels==1,1], color
    ="red",
229             alpha=0.7, label="Type 2 (predicted)")
230
231 plt.xlabel(r"$x_1$")
232 plt.ylabel(r"$x_2$")
233 plt.legend(loc="lower right", frameon=False)
234 plt.tick_params(axis="both", which="both", direction="in")
235 plt.savefig(f"class.pdf", dpi=1080)
236 plt.show()
237
238 # compute accuracy and build confusion matrix
239 acc = accuracy_score(z_true, predicted_labels)
240 cm = confusion_matrix(z_true, predicted_labels)
241
242 print(f"\nClassification accuracy: {acc:.3f}")
243 print(f"\nConfusion matrix:\n", cm)

```

Listing 1: *gmm.py*

```

1 1.
2 x: [[ 2.517704588970049 -0.6704820620140608]
3 [ 2.286594412408074 -0.9844312171306702]
4 [ 1.9960242828701187 -1.1947318652011147]
5 ...
6 [ 1.0688979908502234 -1.3148043634736226]
7 [ 1.940267350973554 -0.1494367115551481]
8 [ 1.7265282647654883 -0.3770063494557934]]
9
10 Eigen values: [2.44339811320566 0.5566018867943396]
11
12 Eigen vectors: [[-0.8746424812468178 0.4847685323929453]
13 [-0.4847685323929453 -0.8746424812468178]]
14
15 Width: 3.1262745325423102
16
17 Height: 1.492115125309491
18
19 Angle: 28.997308395958242 degree
20
21 2.
22 Maximum likelihood: mu_hat = [ 2.014655285377038 -1.0132083392419486]
23
24 Maximum likelihood: Sigma_hat = [[2.069533458212539 0.7855473289101127]
25 [0.7855473289101127 0.9810586095342764]]
26
27 3.
28 GMM w/ one component: mu_gmm = [ 2.014655285377037 -1.0132083392419482]
29
30 GMM w/ one component: Sigma_gmm = [[2.0695344582125386 0.7855473289101127]
31 [0.7855473289101127 0.9810596095342764]]
32
33 mu_error: 9.930136612989092e-16
34
35 Sigma_error: 1.0000000000287557e-06
36
37 4.
38 x (new): [[-5.8688379488870535e-01 -2.0347950258630947e+00]
39 [-1.3568660671935939e-01 -2.3019255565739227e-01]
40 [-2.4897321278945261e-01 -3.0313846599294836e+00]
41 ...
42 [ 1.7043925473325234e+00 -1.0924208747152311e+00]
43 [ 3.6037557851935631e-03 -1.9314825003720597e+00]
44 [ 4.0670328613369993e+00 -1.0552435599485150e+00]]
45
46 Eigen values (new): [2.4809533423908077 0.5696407253560073]
47
48 Eigen vectors (new): [[-0.8858585514333069 0.4639554147248238]
49 [-0.4639554147248238 -0.8858585514333069]]
50
51 Width (new): 3.150208464461238
52
53 Height (new): 1.509490941153351
54
55 Angle (new): 27.64263921232103 degree
56
57 2.
58 For K=1,

```

```

59 Mean: [[3.3043244939443674 2.3696992901480693]]
60
61 Covariance: [[[3.6926089015268726 1.561316587647234 ]
62 [1.561316587647234 2.25828069278701 ]]]
63
64 For K=2,
65 Mean: [[ 0.0887631709875105 -0.0210976144553744]
66 [ 4.0816341486534675 2.9476355599773143]]
67
68 Covariance: [[[ 1.0761406229476318 0.476672845843364 ]
69 [ 0.476672845843364 1.229744902269525 ]]
70
71 [[ 1.2214003949426913 -0.4841133862236404]
72 [-0.4841133862236405 0.7911739159757286]]]
73
74 K=1: log-likelihood = -3725.4576335585434208, Bayesian information criterion =
75 7485.4540435119979520
76
77 K=2: log-likelihood = -3200.4613040281610665, Bayesian information criterion =
78 6476.9079161251256664
79
80 3.
81 For K = 2,
82
83 Weights: [0.1946743731658157 0.8053256268341843]
84
85 Means: [[ 0.0887631709875105 -0.0210976144553744]
86 [ 4.0816341486534675 2.9476355599773143]]
87
88 Covariances: [[[ 1.0761406229476318 0.476672845843364 ]
89 [ 0.476672845843364 1.229744902269525 ]]
90
91 [[ 1.2214003949426913 -0.4841133862236404]
92 [-0.4841133862236405 0.7911739159757286]]]
93
94 5.
95 Classification accuracy: 0.998
96
97 Confusion matrix:
[[184 1]
[ 1 814]]

```

Listing 2: Output terminal for *gmm.py*

III. CHAPTER 4: POLYNOMIAL REGRESSION WITH REGULARIZATION

1. Ridge implementation, diagnostics, and interpretation

1. • For training and testing data, please refer to listing 3 and 4.
- For $\hat{\omega}_\lambda$, please refer to listing 3 and 4.
- Train and test MSE , $\kappa(A^T A)$, and $\kappa(A^T A + \lambda \Gamma^T \Gamma)$ are reported in listing 4.

Below is a representative example of how ridge regression affect the condition number for $M = 6$.

Without regularization:

$$\kappa(A^T A) = 507514157.93791586$$

With regularization for $\lambda = \{10^{-6}, 10^{-4}, 10^{-2}, 10^0, 10^2\}$:

$$\kappa(A^T A + \lambda \Gamma^T \Gamma) = \{117405576.39922069, 1522812.5394117208, 15273.969715717929, 153.2201656595726, 3.9522336795648543\}$$

We can see that with higher value of λ , condition number becomes smaller. So, the linear system becomes well-condition and numerically more stable with greater value of regularization term.

- Test MSE generally increases with higher value of λ as evident from figure 6. The increment is steeper for higher M . For $M = 3, 8$ and 9 , MSE becomes smaller when

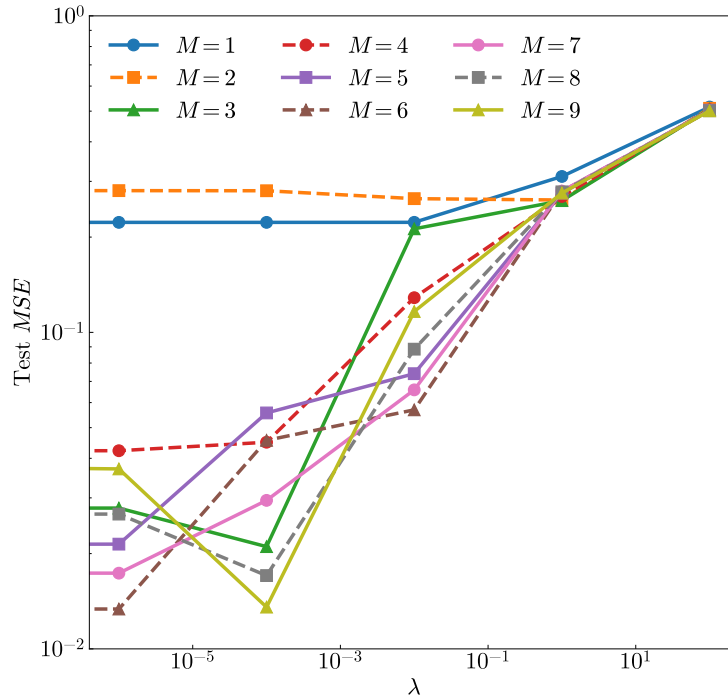


Figure 6: Test MSE vs. λ .

$\lambda = 10^{-4}$ from $\lambda = 10^{-6}$, but then it rises most steeply. High λ penalizes the co-efficients

to great extent inducing high bias and underfitting. This is particularly true for $M \geq 3$. As a result, MSE increases for these. For low order polynomial $M \leq 2$, regularization term has very little effect, till it becomes really large, e.g., $\lambda = 10^2$.

- Without regularization, condition number increases somewhat proportionately with M as can be seen from figure 7.

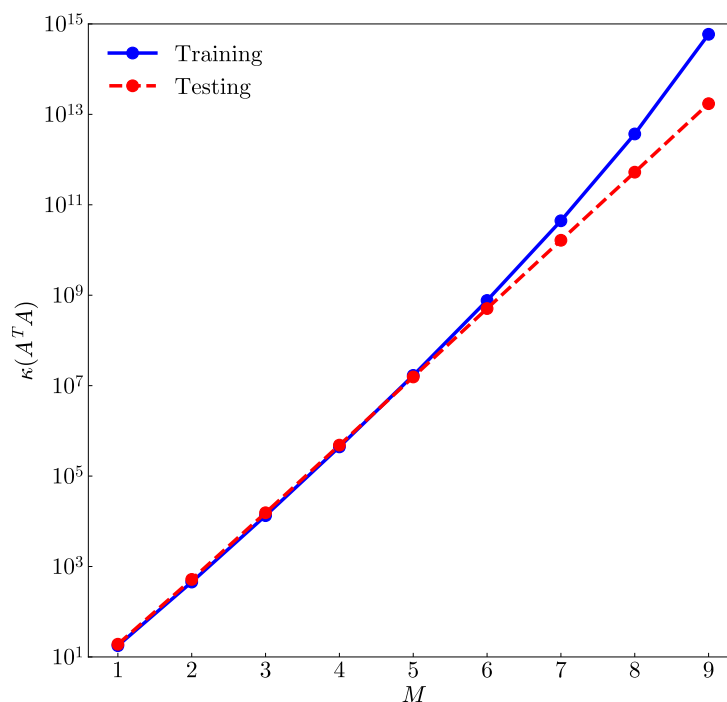
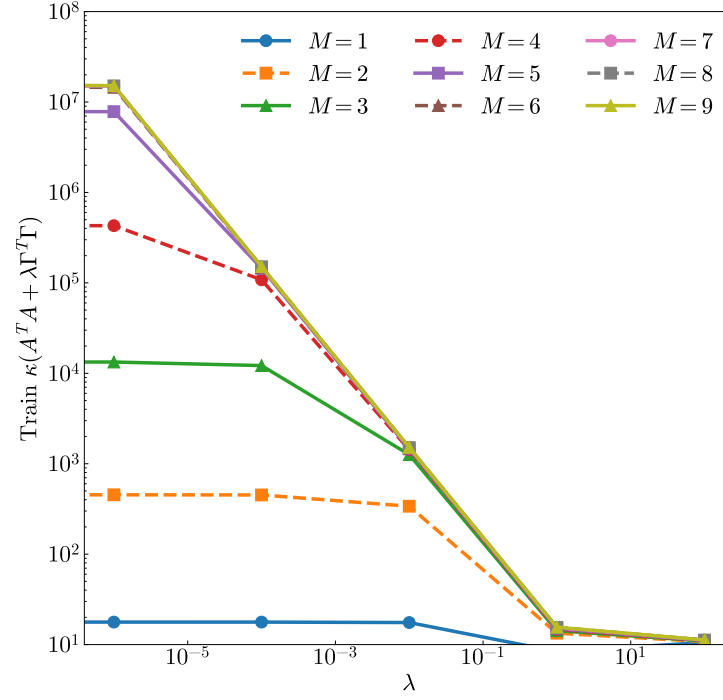
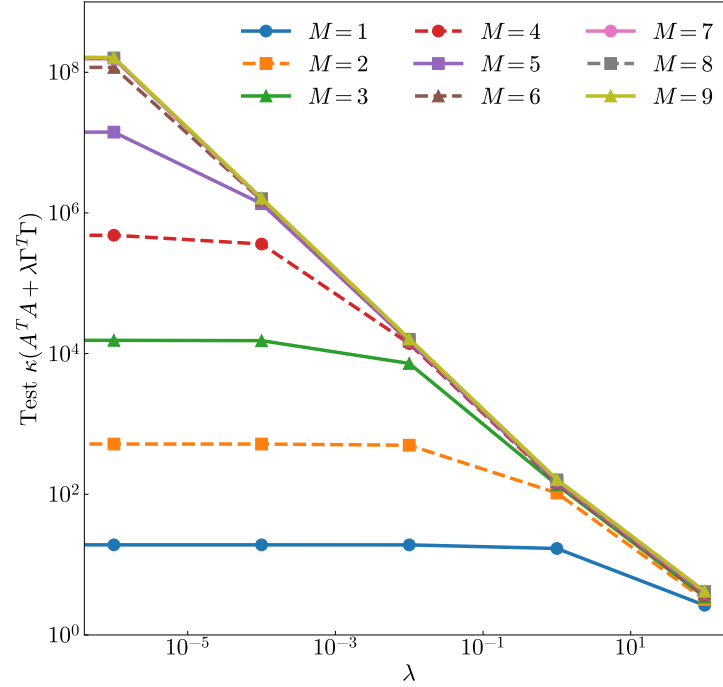


Figure 7: Unregularized condition number with respect to different M .

Now if we look into figure 8, both train and test regularized condition number decreases with higher value of λ . This is again echoing the same message as we got from the comparison of unregularized and regularized example from point-3 with $M = 6$. The linear system becomes well-conditioned with higher value of regularized term parameter.



(a)



(b)

Figure 8: Regularized condition number for (a) training and (b) testing.

2. The verification of closed form ridge regression with `scikit-learn` has been done in listing 3, and shown in 4 in the form of $L2$ norm of error. It can be observed that most of the error

are $< 10^{-10}$. Relatively larger error shows up when regularization is not done, and that is related to the different methods `scikit-learn` (Cholesky, SVD, or other) can use for solving linear system based on the size of the system and conditioning, and the operations might not be the same as `np.linalg.solve()`. If the operations are different, then the accumulated round-off error can come out to be different causing a large difference between the closed form and `scikit-learn` solutions.

3. With higher λ , the penalization term penalizes large co-efficients forcing them to be as small as possible. As a result, curve becomes smoother and less sensitive towards noise, i.e., the variance reduces. However, the model underfits, deviating the predicted value from true value, which leads to increased bias. If we see figure 6, we can understand the effect of underfitting and increased bias with higher λ as MSE increases drastically.

If λ is too small, it introduces high variance and overfitting for higher M . That is why as M increases, it is desirable to increase λ to ensure the ill-conditioning and overfitting is remedied. That is why optimal λ^* is high for higher M , but it must be ensured that it is not as high that it underfits the model. For low M , the system has less chance to be ill-conditioned and is already smooth, so they require very little regularization, lower λ . This can also be checked from figure 6, where we can see that the regularization has very little impact on MSE . This is why the optimal λ^* differs across M and one has to find a sweet spot that does not induce high bias or high variance based on M .

2. Model selection over polynomial degree and regularization

1. (M, λ) that minimizes test MSE along with the minimized test MSE :

$$(\hat{M}, \hat{\lambda}) = (6, 10^{-6}), \quad MSE_{minimized} = 0.013362127882421209$$

2. The co-efficient vectors are given below.

Best fit $(\hat{M}, \hat{\lambda}) = (6, 10^{-6})$:

$$\hat{\omega} = \begin{pmatrix} -0.08958942 \\ 8.47143248 \\ -7.40357783 \\ -40.30544707 \\ 29.78715023 \\ 46.21868656 \\ -36.71097017 \end{pmatrix}$$

Poorly conditioned $(M, \lambda) = (7, 0)$:

$$\hat{\omega} = \begin{pmatrix} -0.0854431228 \\ 8.45284633 \\ -6.55162206 \\ -63.4142787 \\ 170.700841 \\ -294.806939 \\ 323.931451 \\ -139.156624 \end{pmatrix}$$

Overly penalized $(M, \lambda) = (7, 10^0)$:

$$\hat{\omega} = \begin{pmatrix} 0.45998642 \\ -0.42911245 \\ -0.45704387 \\ -0.33176584 \\ -0.20989608 \\ -0.11739408 \\ -0.05236374 \\ -0.00827713 \end{pmatrix}$$

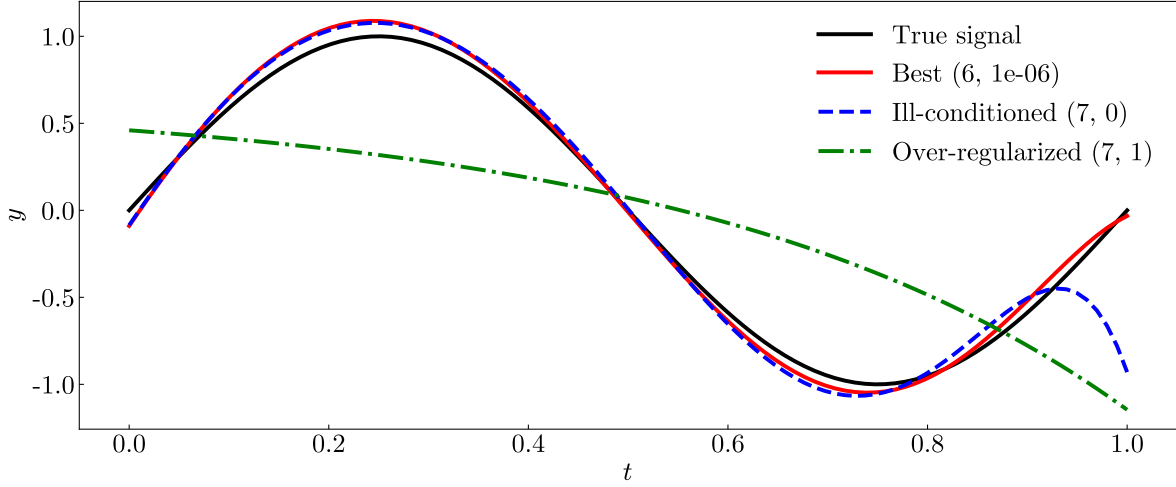


Figure 9: Comparison of the three different fit with true noise-free signal.

We can clearly see from the co-efficient vectors and figure 9 that overly penalized case enforces the co-efficient for higher degree term to be very small, which translates to over-smoothing, increased bias and classic underfitting. This is the worst fit of the three, which suggests that penalizing with high regularization parameter ($\lambda \gg$) can be a disaster.

For poorly conditioned system, the co-efficients for higher degree terms are very big because of no penalization ($\lambda = 0$), and that translates to classic overfitting of the true data. The oscillation near the end of data completely throws the model off the balance despite it doing well for previous data. This is an example of high variance in the model which has the propensity to induce such oscillations towards the either ends of the curve.

The best fit shows a balance of bias and variance, and retains its pattern throughout the data faithfully. The predicted value has some error towards the peak of the true signal, but that is a trade-off that we have to accept in order to faithfully represent the true signal's characteristics. This is achieved with a balanced choice of the regularized parameter ($\lambda = 10^{-6}$). This suggests that the parameter needs to be chosen in such a way that it ensures a good balance between bias and variance.

```

1 import pandas as pd
2 import numpy as np
3 import matplotlib.pyplot as plt
4 import matplotlib as mpl
5 from sklearn.linear_model import Ridge
6
7 def generate_data(scale_noise, N, seed=56):
8     """ Generate a noisy time series dataset {t_i, y_i}_{i=1}^N.
9     Parameters
10    -----
11    A : float
12    Amplitude of the signal (A >= 0)
13    N : int
14    Number of data points. Time points uniformly sampled from [0, 2pi]
15    seed : int or None, optional
16    Random seed for reproducibility """
17
18    rng = np.random.default_rng(seed)
19    t = np.linspace(0.0, 1.0, N)
20    dt = (2*np.pi) / (N - 1)
21    A=np.sqrt(np.pi/dt)
22    s_hat = np.sqrt(dt / np.pi) * np.sin(2*np.pi*t)
23    # ||s_hat||_2 == 1 exactly on this grid
24    s = A * s_hat
25    n = rng.normal(loc=0.0, scale=scale_noise, size=N)
26    y = s + n
27    return t, y, s, n, s_hat, dt
28
29 # ===== 1. Ridge implementation, diagnostics, and interpretation =====
30
31 # 1. Implementation and comparison
32 # generate testing and training data
33 x_data,y_data,s,n,s_hat, dt = generate_data(.1,100)
34 t_train = x_data[:10]
35 y_train = y_data[:10]
36 s_train = s[:10]
37 plt.plot(t_train,y_train,'bo')
38 plt.plot(t_train,s_train,'r--')
39 plt.plot(x_data,s,'k--')
40 plt.show()
41 print("1. Implementation and comparison")
42 print("\nTraining data (t,y):\n", np.column_stack((t_train, y_train)))
43
44 # generate testing data
45 # TODO for YOU: Write code to remove the training data below
46 # t_test and y_test will have 90 data points
47
48 t_test = np.delete(x_data, np.arange(0, len(x_data), 10))
49 y_test = np.delete(y_data, np.arange(0, len(y_data), 10))
50 print("\nTesting data (t, y):\n", np.column_stack((t_test, y_test)))
51
52 # function to construct Vandermonde matrix
53 def vandermonde(t, M):
54     return np.vstack([t**i for i in range(M+1)]).T
55
56 # function to construct  $\gamma$  matrix
57 def gamma(M):
58     g = np.ones(M+1)

```

```

59     g[0] = 0.0
60     return np.diag(g)
61
62 M = np.array([1, 2, 3, 4, 5, 6, 7, 8, 9]) # polynomial orders
63 lambda_ = np.array([0, 1e-6, 1e-4, 1e-2, 1e0, 1e2]) # regularization factors
64
65 omega_train_list = {} # omega for training data
66 mse_train_list = {} # training MSE
67 mse_test_list = {} # testing MSE
68 cond_no_train_list = {} # training condition no. w/o regularization factor
69 cond_no_ridge_train_list = {} # training condition no. w/ regularization
    factor
70 cond_no_test_list = {} # testing condition no. w/o regularization factor
71 cond_no_ridge_test_list = {} # testing condition no. w/ regularization factor
72
73 for i in M:
74     A_train = vandermonde(t_train, i)
75     A_test = vandermonde(t_test, i)
76     for j in lambda_:
77         omega_train = np.linalg.solve(((A_train.T @ A_train) +
78                                         j * (gamma(i).T @ gamma(i))), (A_train.T @
79                                         y_train))
80         omega_train_list[(i, j)] = omega_train
81         y_train_predict = A_train @ omega_train
82         y_test_predict = A_test @ omega_train
83         mse_train = np.mean((abs(y_train_predict - y_train))**2)
84         mse_train_list[(i, j)] = mse_train # update traing MSE list
85         mse_test = np.mean((abs(y_test_predict - y_test))**2)
86         mse_test_list[(i, j)] = mse_test # update testing MSE list
87         # compute and update condition no. lists
88         cond_no_train = np.linalg.cond(A_train.T @ A_train, 2)
89         cond_no_train_list[(i, j)] = cond_no_train
90         cond_no_ridge_train = np.linalg.cond((A_train.T @ A_train + j * gamma(
91             i).T @ gamma(i))), 2)
92         cond_no_ridge_train_list[(i, j)] = cond_no_ridge_train
93         cond_no_test = np.linalg.cond(A_test.T @ A_test, 2)
94         cond_no_test_list[(i, j)] = cond_no_test
95         cond_no_ridge_test = np.linalg.cond((A_test.T @ A_test + j * gamma(i).
96             T @ gamma(i))), 2)
97         cond_no_ridge_test_list[(i, j)] = cond_no_ridge_test
98
99 print("\n$omega$:", omega_train_list)
100 print("\nMSE (training):", mse_train_list)
101 print("\nMSE (testing):", mse_test_list)
102 print("\nCondition no. w/o regularization (training):", cond_no_train_list)
103 print("\nCondition no. w/ regularization (training):",
104       cond_no_ridge_train_list)
105 print("\nCondition no. w/o regularization (testing):", cond_no_test_list)
106 print("\nCondition no. w/ regularization (testing):", cond_no_ridge_test_list)
107
108 df = pd.DataFrame([[M_val, lam, mse_train_list[(M_val, lam)],
109                    mse_test_list[(M_val, lam)],
110                    cond_no_train_list[(M_val, lam)],
111                    cond_no_ridge_train_list[(M_val, lam)],
112                    cond_no_test_list[(M_val, lam)], cond_no_ridge_test_list[(
113                        M_val, lam)]]
114                    for M_val in M for lam in lambda_],
115                  columns=["M", "$\lambda$", "MSE_train", "MSE_test", "$\kappa(A^TA)_train$",
116                          "$\kappa(A^TA+\lambda\gamma^T\gamma)_train$", "$\kappa(A^TA)_test$",

```

```

112     "$kappa(A^TA+\\lambda\\gamma^T\\gamma)_test$"]
113 print("\\nTable for all combinations:\\n", df)
114
115 # parameters for plotting
116 plt.rcParams["font.family"] = "serif"
117 plt.rcParams["font.serif"] = ["CMU Serif"]
118 plt.rcParams["mathtext.fontset"] = "cm"
119 plt.rcParams["font.size"] = 20
120 mpl.rcParams["axes.unicode_minus"] = False
121
122 # mse plots
123 fig, ax = plt.subplots(figsize=(10, 10))
124 markers = ["o", "s", "^"]
125 linestyle = ["-", "--"]
126
127 for i, M_val in enumerate(M):
128     subset = df[df["M"] == M_val]
129     ax.loglog(subset["$\\lambda$"], subset["MSE_test"],
130              marker=markers[i % len(markers)], markersize=10,
131              linestyle=linestyle[i % len(linestyle)], linewidth=3,
132              label=fr"$M={M_val}$")
133
134 plt.xlabel(r"$\\lambda$")
135 plt.ylabel(r"Test $MSE$")
136 plt.ylim(1e-2, 1e0)
137 plt.legend(frameon=False, loc="best", ncol=3)
138 plt.tick_params(axis="both", which="both", direction="in")
139 plt.savefig("ridge_mse.pdf", dpi=1080)
140 plt.show()
141
142 # condition no. plot w/o regularization
143 fig, ax = plt.subplots(figsize=(10, 10))
144
145 subset = df[df["$\\lambda$"] == 0].sort_values("M")
146
147 ax.semilogy(subset["M"], subset["$kappa(A^TA)_train$"], "-o", markersize=10,
148             linewidth=3, color="blue", label="Training")
149 ax.semilogy(subset["M"], subset["$kappa(A^TA)_test$"], "--o", markersize=10,
150             linewidth=3, color="red", label="Testing")
151
152 plt.xlabel(r"$M$")
153 plt.ylabel(r"$\\kappa(A^TA)$")
154 plt.ylim(1e1, 1e15)
155 plt.legend(frameon=False, loc="upper left")
156 plt.tick_params(axis="both", which="both", direction="in")
157 plt.savefig("cond.pdf", dpi=1080)
158 plt.show()
159
160 # condition no. plot w/ regularizations
161 fig, ax = plt.subplots(figsize=(10, 10))
162 markers = ["o", "s", "^"]
163 linestyle = ["-", "--"]
164
165 for i, M_val in enumerate(M):
166     subset = df[df["M"] == M_val]
167     ax.loglog(subset["$\\lambda$"], subset["$kappa(A^TA+\\lambda\\gamma^T\\gamma)_train$"],

```

```

168         label=fr"$M={M_val}$")
169
170 plt.xlabel(r"$\lambda$")
171 plt.ylabel(r"Train $\kappa(A^T A + \lambda \Gamma^T \Gamma)$")
172 plt.ylim(1e1, 1e8)
173 plt.legend(frameon=False, loc="upper right", ncol=3)
174 plt.tick_params(axis="both", which="both", direction="in")
175 plt.savefig("train_ridge_cond.pdf", dpi=1080)
176 plt.show()
177
178 fig, ax = plt.subplots(figsize=(10, 10))
179 markers = ["o", "s", "^"]
180 linestyle = ["-", "--"]
181
182 for i, M_val in enumerate(M):
183     subset = df[df["M"] == M_val]
184     ax.loglog(subset["$\\lambda$"], subset["$\\kappa(A^T A + \\lambda \\gamma^T \\gamma)_test$"],
185              marker=markers[i % len(markers)], markersize=10,
186              linestyle=linestyle[i % len(linestyle)], linewidth=3,
187              label=fr"$M={M_val}$")
188 plt.xlabel(r"$\lambda$")
189 plt.ylabel(r"Test $\kappa(A^T A + \lambda \Gamma^T \Gamma)$")
190 plt.ylim(1e0, 1e9)
191 plt.legend(frameon=False, loc='upper right', ncol=3)
192 plt.tick_params(axis="both", which="both", direction="in")
193 plt.savefig("test_ridge_cond.pdf", dpi=1080)
194 plt.show()
195
196 # 2. Equivalence check with scikit-learn
197 diff = []
198
199 print("\n2. Equivalence check with scikit-learn")
200 for M_val in M:
201     A_train = vandermonde(t_train, M_val)
202     I = np.eye(M_val + 1)
203     for lam in lambda_:
204         # closed form solution
205         omega_closed = np.linalg.solve((A_train.T @ A_train) +
206                                       lam * (I.T @ I), A_train.T @ y_train)
207
208         # scikit-learn solution
209         ridge = Ridge(alpha=lam, fit_intercept=False, solver='auto')
210         ridge.fit(A_train, y_train)
211         omega_sklearn = ridge.coef_
212
213         # compute l2 norm
214         diff_ = np.linalg.norm(omega_closed - omega_sklearn)
215         diff.append([M_val, lam, diff_])
216
217     print(f"\nM={M_val:2d}, lambda={lam:8.1e}, error={diff_:2e}")
218
219 # dataframe
220 df_diff = pd.DataFrame(diff, columns=["M", "$\lambda$", "l2"])
221 print("\nCoefficient L2-norm differences across all (M, $\lambda$):\n")
222 print(df_diff)
223
224 # ===== 2. Model selection over polynomial degree and regularization =====
225

```

```

226 # 1. Grid search over (M,  $\lambda$ )
227 M_hat, lambda_hat = min(mse_test_list, key=mse_test_list.get)
228 min_mse_test = mse_test_list[M_hat, lambda_hat]
229
230 print(f"\n1. Grid search over (M,  $\lambda$ )")
231 print(f"\nBest (M_hat, Lambda) = ({M_hat}, {lambda_hat})")
232 print(f"\nMinimum Test MSE = {min_mse_test}")
233
234 # 2. Final reflections
235 cases = [
236     ("Best", M_hat, lambda_hat),
237     ("Ill-conditioned", 7, 0),
238     ("Over-regularized", 7, 1e0)
239 ]
240
241 coeffs_list = {}
242
243 print(f"\n2. Final reflections")
244
245 # pick the (M,  $\lambda$ ) for comparison
246 for label, M_val, lam in cases:
247     coeffs_list[label] = omega_train_list[(M_val, lam)]
248     print(f"\n{label} coefficients (M={M_val},  $\lambda$ = $\lambda$ ={lam:g}):")
249     print(coeffs_list[label])
250
251 # noise-free true signal
252 _, _, s_true, _, _, _ = generate_data(0.0, 100, seed=56)
253
254 # plot for comparison
255 fig, ax = plt.subplots(figsize=(15, 6))
256
257 ax.plot(x_data, s_true, "k-", linewidth=3, label="True signal")
258
259 colors = ["red", "blue", "green"]
260 linestyles = ["-", "--", "-."]
261
262 for (label, M_val, lam), color, ls in zip(cases, colors, linestyles):
263     A_plot = vandermonde(x_data, M_val)
264     y_fit = A_plot @ coeffs_list[label]
265     ax.plot(x_data, y_fit, color=color, linestyle=ls, linewidth=3,
266            label=f"{label} (M={M_val},  $\lambda$ = $\lambda$ ={lam:g})")
267
268 plt.xlabel(r"$t$")
269 plt.ylabel(r"$y$")
270 plt.legend(frameon=False, loc="upper right")
271 plt.tick_params(axis="both", which="both", direction="in")
272 plt.savefig("signal_fit.pdf", dpi=1080)
273 plt.show()

```

Listing 3: *ridge.py*

```

1 1. Implementation and comparison
2
3 Training data (t, y):
4 [[ 0.          -0.08499407]
5  [ 0.1010101   0.64733005]
6  [ 0.2020202   1.05181989]
7  [ 0.3030303   0.98179583]
8  [ 0.4040404   0.66274571]
9  [ 0.50505051  -0.07132869]
10 [ 0.60606061  -0.66085845]
11 [ 0.70707071  -1.06338572]
12 [ 0.80808081  -0.9015869 ]
13 [ 0.90909091  -0.47937759]]
14
15 Testing data (t, y):
16 [[ 0.01010101  0.095618 ]
17  [ 0.02020202  0.30549674]
18  [ 0.03030303  0.27718516]
19  [ 0.04040404  0.28830727]
20  [ 0.05050505  0.46080282]
21  [ 0.06060606  0.44452901]
22  [ 0.07070707  0.63791978]
23  [ 0.08080808  0.35246993]
24  [ 0.09090909  0.55317597]
25  [ 0.11111111  0.57540486]
26  [ 0.12121212  0.69204348]
27  [ 0.13131313  0.6287832 ]
28  [ 0.14141414  0.64133984]
29  [ 0.15151515  0.93655855]
30  [ 0.16161616  0.60970634]
31  [ 0.17171717  0.72579539]
32  [ 0.18181818  0.86814952]
33  [ 0.19191919  0.83364087]
34  [ 0.21212121  1.03648661]
35  [ 0.22222222  1.01153419]
36  [ 0.23232323  1.14854167]
37  [ 0.24242424  1.11652099]
38  [ 0.25252525  1.11487025]
39  [ 0.26262626  1.03486301]
40  [ 0.27272727  0.99333582]
41  [ 0.28282828  1.06649211]
42  [ 0.29292929  1.06171274]
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48  [ 0.36363636  0.72778199]
49  [ 0.37373737  0.78754805]
50  [ 0.38383838  0.67999822]
51  [ 0.39393939  0.61619001]
52  [ 0.41414141  0.50515954]
53  [ 0.42424242  0.52153018]
54  [ 0.43434343  0.28565485]
55  [ 0.44444444  0.51476062]
56  [ 0.45454545  0.22247404]
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106
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127      -0.11739408, -0.05236374, -0.00827713]), (7, 100.0): array([
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129      7.54510095e+02, -1.63178503e+03,  2.03971983e+03, -1.29468748e+03,
130      3.17770964e+02]), (8, 1e-06): array([ -0.08615891,  8.7863877 ,
-12.99165873, -16.38121648,
131      3.55068973,  18.04569895,  17.23284674,  2.41985936,
132      -21.29447286]), (8, 0.0001): array([ -0.06832276,  9.30339119,

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133         -18.74152461, -5.37864909,
134         6.65863436, 9.938852, 6.60400447, -0.13089784,
135         -7.90884346]], (8, 0.01): array([ 0.42859457, 2.33224272,
136         -4.51855987, -3.13044096, -0.91207784,
137         0.72057211, 1.69669712, 2.19173531, 2.37688458]), (8, 1.0): array([
138         0.46024244, -0.42980936, -0.45826299, -0.33322199, -0.21143069,
139         -0.11892075, -0.05383594, -0.00967079, 0.0195075 ]), (8, 100.0): array
140         ([ 0.02620557, -0.01499511, -0.01506, -0.01262136, -0.01019196,
141         -0.00820112, -0.0066437, -0.00543545, -0.00449369]), (9, 0.0): array
142         ([-8.49935269e-02, -3.27648701e+01, 1.03824219e+03, -1.03879742e
143         +04,
144         5.33810068e+04, -1.59342687e+05, 2.86104933e+05, -3.04371861e+05,
145         1.76702113e+05, -4.31160604e+04]), (9, 1e-06): array([ -0.08689569,
146         8.92113169, -14.27388064, -13.41613075,
147         4.29170421, 13.35759818, 12.35062437, 5.34641257,
148         -3.98552164, -13.45642539]), (9, 0.0001): array([ -0.06727238,
149         9.14152576, -17.77551295, -6.05787573,
150         5.10066393, 9.081699, 7.54903078, 3.08772435,
151         -2.40401567, -7.79971759]), (9, 0.01): array([ 0.42272997, 2.322687
152         , -4.36441073, -3.06238671, -1.0029335,
153         0.47461423, 1.32506153, 1.72841883, 1.85269188, 1.816474 ]), (9,
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155         -0.21382411,
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158         -0.01018237,
159         -0.00819231, -0.00663567, -0.00542816, -0.00448709, -0.00374667])}]
160
161 MSE (training): {(1, 0.0): 0.27073288909194354, (1, 1e-06):
162 0.27073288909234483, (1, 0.0001): 0.27073289310345405, (1, 0.01):
163 0.2707720770906607, (1, 1.0): 0.3545468710021419, (1, 100.0):
164 0.5503073352430806, (2, 0.0): 0.23133288031654056, (2, 1e-06):
165 0.23133288033543628, (2, 0.0001): 0.23133306802503034, (2, 0.01):
166 0.23239419334679398, (2, 1.0): 0.2936344906347173, (2, 100.0):
167 0.5456413991349919, (3, 0.0): 0.006521765184228492, (3, 1e-06):
168 0.00652198737491233, (3, 0.0001): 0.00837558444932197, (3, 0.01):
169 0.20527662605749836, (3, 1.0): 0.27984623261605035, (3, 100.0):
170 0.5424190489982516, (4, 0.0): 0.004689033380580246, (4, 1e-06):
171 0.004689750410450222, (4, 0.0001): 0.0053854390750167885, (4, 0.01):
172 0.15196831328445443, (4, 1.0): 0.2789739042905329, (4, 100.0):
173 0.5403477737449263, (5, 0.0): 0.001127982418387338, (5, 1e-06):
174 0.0021024362826733345, (5, 0.0001): 0.006416159311522294, (5, 0.01):
175 0.11093727362946038, (5, 1.0): 0.2804542007363015, (5, 100.0):
176 0.5390234911746371, (6, 0.0): 0.0006273934530143964, (6, 1e-06):
177 0.0009639024324000196, (6, 0.0001): 0.005353219860754832, (6, 0.01):
178 0.08829109466639389, (6, 1.0): 0.2814963019244499, (6, 100.0):
179 0.5381641994522264, (7, 0.0): 0.0006049563056163806, (7, 1e-06):
180 0.0006884547510555836, (7, 0.0001): 0.0037819831459206853, (7, 0.01):
181 0.07812673336176454, (7, 1.0): 0.28168632608569505, (7, 100.0):
182 0.5375948849228811, (8, 0.0): 0.0006022598739992099, (8, 1e-06):
183 0.0006172325489378455, (8, 0.0001): 0.0025103931650422677, (8, 0.01):
184 0.0745949645894507, (8, 1.0): 0.28122052407527365, (8, 100.0):
185 0.5372093532130965, (9, 0.0): 4.818198085563335e-10, (9, 1e-06):
186 0.0006085594474656156, (9, 0.0001): 0.0016956592073576534, (9, 0.01):
187 0.07409067937027043, (9, 1.0): 0.28036961174950115, (9, 100.0):
188 0.5369427468444984}
189
190 MSE (testing): {(1, 0.0): 0.22261110362410202, (1, 1e-06):
191 0.22261110635622774, (1, 0.0001): 0.22261138092837973, (1, 0.01):

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151
152 Condition no. w/o regularization (training): {(1, 0.0): 17.737248092888933,
(1, 1e-06): 17.737248092888933, (1, 0.0001): 17.737248092888933, (1, 0.01):
: 17.737248092888933, (1, 1.0): 17.737248092888933, (1, 100.0):
17.737248092888933, (2, 0.0): 453.31428795133763, (2, 1e-06):
453.31428795133763, (2, 0.0001): 453.31428795133763, (2, 0.01):
453.31428795133763, (2, 1.0): 453.31428795133763, (2, 100.0):
453.31428795133763, (3, 0.0): 13339.252757834696, (3, 1e-06):
13339.252757834696, (3, 0.0001): 13339.252757834696, (3, 0.01):
13339.252757834696, (3, 1.0): 13339.252757834696, (3, 100.0):
13339.252757834696, (4, 0.0): 442460.9052181754, (4, 1e-06):
442460.9052181754, (4, 0.0001): 442460.9052181754, (4, 0.01):
442460.9052181754, (4, 1.0): 442460.9052181754, (4, 100.0):
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16844073.40840483, (5, 0.0001): 16844073.40840483, (5, 0.01):
16844073.40840483, (5, 1.0): 16844073.40840483, (5, 100.0):
16844073.40840483, (6, 0.0): 765246943.950359, (6, 1e-06):
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765246943.950359, (6, 1.0): 765246943.950359, (6, 100.0):
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590145630456648.8, (9, 0.0001): 590145630456648.8, (9, 0.01):
590145630456648.8, (9, 1.0): 590145630456648.8, (9, 100.0):
590145630456648.8}

153
154 Condition no. w/ regularization (training): {(1, 0.0): 17.737248092888933, (1,
1e-06): 17.737227579792254, (1, 0.0001): 17.735197024882076, (1, 0.01):
17.534529534421594, (1, 1.0): 8.383151748716001, (1, 100.0):

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13326.481598240725, (3, 0.0001): 12172.70886340197, (3, 0.01):
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1428.1239060044268, (4, 1.0): 14.684340726195504, (4, 100.0):
11.05434066861605, (5, 0.0): 16844073.40840483, (5, 1e-06):
7822923.186889193, (5, 0.0001): 144812.3062395995, (5, 0.01):
1460.9120827517897, (5, 1.0): 14.986651913795011, (5, 100.0):
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15073306.004044555, (8, 0.0001): 150734.0592951826, (8, 0.01):
1507.7299069289086, (8, 1.0): 15.485194686523528, (8, 100.0):
11.230080149708563, (9, 0.0): 590145630456648.8, (9, 1e-06):
15159936.566786056, (9, 0.0001): 151599.7644476303, (9, 0.01):
1516.3927581144233, (9, 1.0): 15.577731739022951, (9, 100.0):
11.250312536364762}

155 Condition no. w/o regularization (testing): {(1, 0.0): 19.106223493478968, (1,
156 1e-06): 19.106223493478968, (1, 0.0001): 19.106223493478968, (1, 0.01):
19.106223493478968, (1, 1.0): 19.106223493478968, (1, 100.0):
19.106223493478968, (2, 0.0): 518.3247156838922, (2, 1e-06):
518.3247156838922, (2, 0.0001): 518.3247156838922, (2, 0.01):
518.3247156838922, (2, 1.0): 518.3247156838922, (2, 100.0):
518.3247156838922, (3, 0.0): 15453.409539349419, (3, 1e-06):
15453.409539349419, (3, 0.0001): 15453.409539349419, (3, 0.01):
15453.409539349419, (3, 1.0): 15453.409539349419, (3, 100.0):
15453.409539349419, (4, 0.0): 483506.95964456553, (4, 1e-06):
483506.95964456553, (4, 0.0001): 483506.95964456553, (4, 0.01):
483506.95964456553, (4, 1.0): 483506.95964456553, (4, 100.0):
483506.95964456553, (5, 0.0): 15576875.806916751, (5, 1e-06):
15576875.806916751, (5, 0.0001): 15576875.806916751, (5, 0.01):
15576875.806916751, (5, 1.0): 15576875.806916751, (5, 100.0):
15576875.806916751, (6, 0.0): 507514157.93791586, (6, 1e-06):
507514157.93791586, (6, 0.0001): 507514157.93791586, (6, 0.01):
507514157.93791586, (6, 1.0): 507514157.93791586, (6, 100.0):
507514157.93791586, (7, 0.0): 16416963221.690588, (7, 1e-06):
16416963221.690588, (7, 0.0001): 16416963221.690588, (7, 0.01):
16416963221.690588, (7, 1.0): 16416963221.690588, (7, 100.0):
16416963221.690588, (8, 0.0): 526138212360.06726, (8, 1e-06):
526138212360.06726, (8, 0.0001): 526138212360.06726, (8, 0.01):
526138212360.06726, (8, 1.0): 526138212360.06726, (8, 100.0):
526138212360.06726, (9, 0.0): 17234710195847.965, (9, 1e-06):
17234710195847.965, (9, 0.0001): 17234710195847.965, (9, 0.01):
17234710195847.965, (9, 1.0): 17234710195847.965, (9, 100.0):
17234710195847.965}

157 Condition no. w/ regularization (testing): {(1, 0.0): 19.106223493478968, (1,
158 1e-06): 19.10622106719703, (1, 0.0001): 19.105980868437282, (1, 0.01):
19.08199246082843, (1, 1.0): 16.961404261076325, (1, 100.0):
2.6451792838145556, (2, 0.0): 518.3247156838922, (2, 1e-06):

```

```

518.3226504337313, (2, 0.0001): 518.1182721658406, (2, 0.01):
498.46409096921354, (2, 1.0): 104.24772742787077, (2, 100.0):
3.1793725472959626, (3, 0.0): 15453.409539349419, (3, 1e-06):
15451.66371493911, (3, 0.0001): 15280.758144376809, (3, 0.01):
7255.702908857381, (3, 1.0): 135.96014308288903, (3, 100.0):
3.4819683571427062, (4, 0.0): 483506.95964456553, (4, 1e-06):
481880.15127956885, (4, 0.0001): 361474.59815095615, (4, 0.01):
13910.423706190382, (4, 1.0): 143.60323838786084, (4, 100.0):
3.6842914558245314, (5, 0.0): 15576875.806916751, (5, 1e-06):
14097391.456519287, (5, 0.0001): 1355131.3306713083, (5, 0.01):
14828.880943341705, (5, 1.0): 148.8798051509931, (5, 100.0):
3.8339619443682857, (6, 0.0): 507514157.93791586, (6, 1e-06):
117405576.39922069, (6, 0.0001): 1522812.5394117208, (6, 0.01):
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3.9522336795648543, (7, 0.0): 16416963221.690588, (7, 1e-06):
154944836.79662007, (7, 0.0001): 1564063.012888165, (7, 0.01):
15642.600206473078, (7, 1.0): 156.92276068406156, (7, 100.0):
4.049999161567223, (8, 0.0): 526138212360.06726, (8, 1e-06):
159586290.01653725, (8, 0.0001): 1596342.7662737397, (8, 0.01):
15963.988048226052, (8, 1.0): 160.15416845668432, (8, 100.0):
4.133439868338479, (9, 0.0): 17234710195847.965, (9, 1e-06):
162487441.82454658, (9, 0.0001): 1624890.1125685496, (9, 0.01):
16249.430491895779, (9, 1.0): 163.02397875475458, (9, 100.0):
4.206349805749418}

```

159

160 2. Equivalence check with scikit-learn

161

162 Coefficient L2-norm differences across all (M, \$\lambda\$):

163

	M	\$\lambda\$	L2
164			
165	0	1	0.000000 1.180183e-15
166	1	1	0.000001 2.234281e-15
167	2	1	0.000100 1.601186e-15
168	3	1	0.010000 6.280370e-16
169	4	1	1.000000 1.110223e-16
170	5	1	100.000000 1.734723e-18
171	6	2	0.000000 1.651249e-14
172	7	2	0.000001 1.546362e-15
173	8	2	0.000100 5.925929e-15
174	9	2	0.010000 6.179030e-15
175	10	2	1.000000 2.001483e-16
176	11	2	100.000000 4.911328e-18
177	12	3	0.000000 3.748011e-12
178	13	3	0.000001 3.077815e-12
179	14	3	0.000100 2.359466e-12
180	15	3	0.010000 3.748890e-14
181	16	3	1.000000 2.543841e-16
182	17	3	100.000000 5.222209e-18
183	18	4	0.000000 1.165418e-10
184	19	4	0.000001 6.354021e-11
185	20	4	0.000100 1.529848e-11
186	21	4	0.010000 3.272221e-14
187	22	4	1.000000 2.676651e-16
188	23	4	100.000000 5.502793e-18
189	24	5	0.000000 1.690115e-08
190	25	5	0.000001 1.350438e-09
191	26	5	0.000100 1.231346e-11
192	27	5	0.010000 9.366574e-14
193	28	5	1.000000 1.520235e-16

```

194 29 5 100.000000 4.925668e-18
195 30 6 0.000000 1.266891e-06
196 31 6 0.000001 3.742331e-09
197 32 6 0.000100 1.236106e-11
198 33 6 0.010000 1.322486e-13
199 34 6 1.000000 1.825338e-16
200 35 6 100.000000 6.329364e-18
201 36 7 0.000000 2.679460e-05
202 37 7 0.000001 8.541492e-10
203 38 7 0.000100 9.051553e-12
204 39 7 0.010000 1.518729e-13
205 40 7 1.000000 2.258674e-16
206 41 7 100.000000 7.961322e-18
207 42 8 0.000000 8.934914e-03
208 43 8 0.000001 2.702463e-09
209 44 8 0.000100 2.718318e-11
210 45 8 0.010000 1.369087e-13
211 46 8 1.000000 3.341178e-16
212 47 8 100.000000 5.818439e-18
213 48 9 0.000000 4.322710e+02
214 49 9 0.000001 2.989578e-09
215 50 9 0.000100 1.409848e-11
216 51 9 0.010000 1.333104e-13
217 52 9 1.000000 2.436777e-16
218 53 9 100.000000 7.256869e-18
219
220 1. Grid search over (M,  $\lambda$ )
221
222 Best (M_hat, Lambda) = (6, 1e-06)
223
224 Minimum Test MSE = 0.013362127882421209
225
226 2. Final reflections
227
228 Best coefficients (M=6,  $\lambda=1e-06$ ):
229 [ -0.08958942  8.47143248 -7.40357783 -40.30544707  29.78715023
230   46.21868656 -36.71097017]
231
232 Ill-conditioned coefficients (M=7,  $\lambda=0$ ):
233 [-8.54431228e-02  8.45284633e+00 -6.55162206e+00 -6.34142787e+01
234   1.70700841e+02 -2.94806939e+02  3.23931451e+02 -1.39156624e+02]
235
236 Over-regularized coefficients (M=7,  $\lambda=1$ ):
237 [ 0.45998642 -0.42911245 -0.45704387 -0.33176584 -0.20989608 -0.11739408
238  -0.05236374 -0.00827713]

```

Listing 4: Output terminal (selected) for *ridge.py*

IV. GMM & REGRESSION FOR MARINE CRAFT DYNAMICS

- The predictor model used in this work is a combination of smooth deterministic terms and harmonic terms. The smooth deterministic terms are expressed in the form of *Legendre* polynomials and the harmonic terms are expressed in the form of sine/cosine wave. The predictor for this problem is written as,

$$\hat{y}(t) = \sum_{i=0}^n \beta_i P_i(\tilde{t}) + \sum_{j=1}^m (a_j \cos(\omega_j \pi \tilde{t}) + b_j \sin(\omega_j \pi \tilde{t})) \quad (1)$$

where, P_i is the *Legendre* polynomial of degree i with corresponding weights β_i , and a_j and b_j are the weights (amplitude) for the harmonic terms with frequency ω_j . This predictor is formulated to capture both the smooth varying trend and the oscillatory responses due to waves.

For improving the condition number of the design matrix, t is normalized and expressed as:

$$\tilde{t} = \frac{2(t - t_{min})}{t_{max} - t_{min}} - 1$$

which conforms to the bound of $[-1, 1]$.

After setting $n = m = 2$ and $\omega \in \{1, 2\}$, the final form of equation (1) stands as,

$$\hat{y}(t) = \sum_{i=0}^2 \beta_i P_i(\tilde{t}) + \sum_{j=1}^2 (a_j \cos(\omega_j \pi \tilde{t}) + b_j \sin(\omega_j \pi \tilde{t})) \quad (2)$$

$\{(t_i, y_i)\}_{i=1}^N$ are split into 70% training and 30% testing data, and the design matrices were formed. The condition number of the design matrices were found to be-

$$\kappa(A^T A)_{train} = 1.1 \times 10^5, \quad \kappa(A^T A)_{test} = 2.86 \times 10^{10}$$

which points to a potential ill-conditioned system. Performing regression to this system to

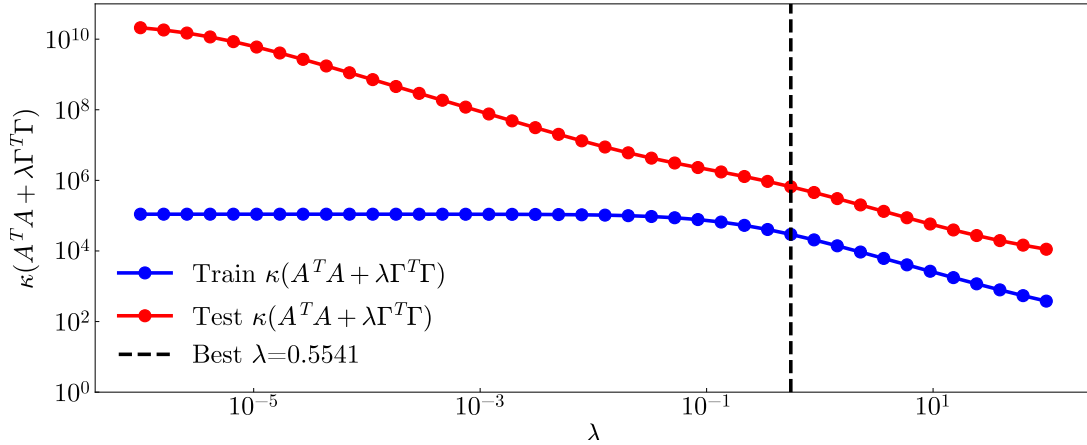


Figure 10: Condition number as a function of λ .

find the optimal weights can result in overfitting of the data. To remedy this, regularization

was performed on $A^T A$ which improved the condition number as can be seen from figure 10 and normal equations were formulated to find out the weights.

$$\hat{\theta} = (A^T A + \lambda \Gamma^T \Gamma)^{-1} A^T y$$

The best weights were picked by doing a grid search to find the value of λ for which the test MSE is minimum. Figure 11 shows the train and test MSE , and how the minimum test MSE was clearly distinguishable. The best weights corresponding to $\lambda = 0.5541$ came out

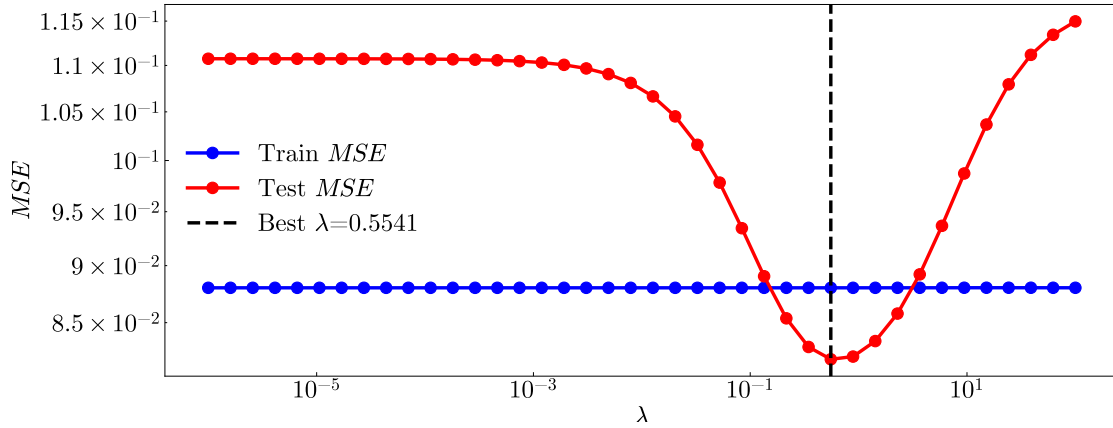


Figure 11: MSE as a function of λ .

to be-

$$\beta_i = \begin{pmatrix} -0.00744026 \\ 1.17051422 \\ -0.46714436 \end{pmatrix}, \quad a_j = \begin{pmatrix} -0.05609375 \\ 0.0089983 \end{pmatrix}, \quad b_j = \begin{pmatrix} -0.07363466 \\ 0.00805816 \end{pmatrix}$$

The model shown in figure 12 is obtained by finding a balance between bias and variance,

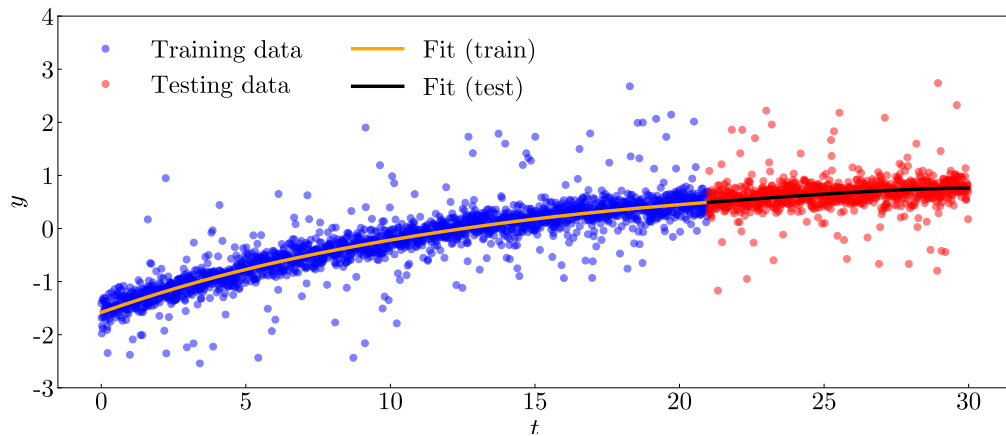


Figure 12: Predicted model via *Ridge* regression.

so that it does not suffer from underfitting due to high λ or overfitting due to ill-conditioned system with unregularized weights.

After building the forecasting model, the noise model was formulated in the form-

$$p(\epsilon) = \sum_{k=1}^2 \pi_k \mathcal{N}(\epsilon | \mu_k, \sigma_k^2) \quad (3)$$

This is a 1D Gaussian mixture model and has two components- one relates to background sea state and another to slamming events. The distribution of training residual was plotted in figure 13. The parameters for the 1D GMM are found to be-

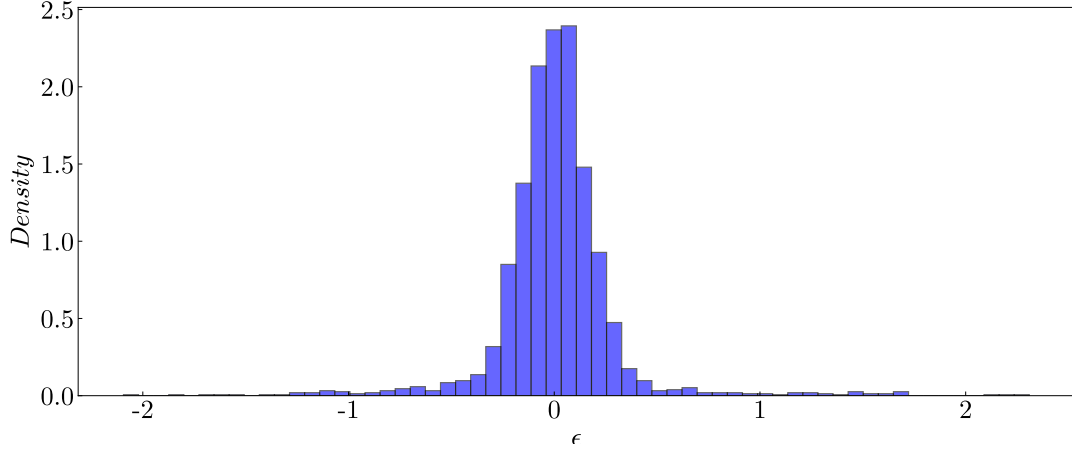


Figure 13: Training residual distribution.

For $k = 1$ (background sea state),

$$\pi_1 = 0.9017, \quad \mu_1 = 0.0061, \quad \sigma_1^2 = 0.0226, \quad \sigma_1 = 0.1502$$

For $k = 2$ (Slamming events),

$$\pi_2 = 0.0983, \quad \mu_2 = 0.0153, \quad \sigma_2^2 = 0.6882, \quad \sigma_2 = 0.8296$$

As expected, figure 14 shows the large variance in the slamming events with probability of

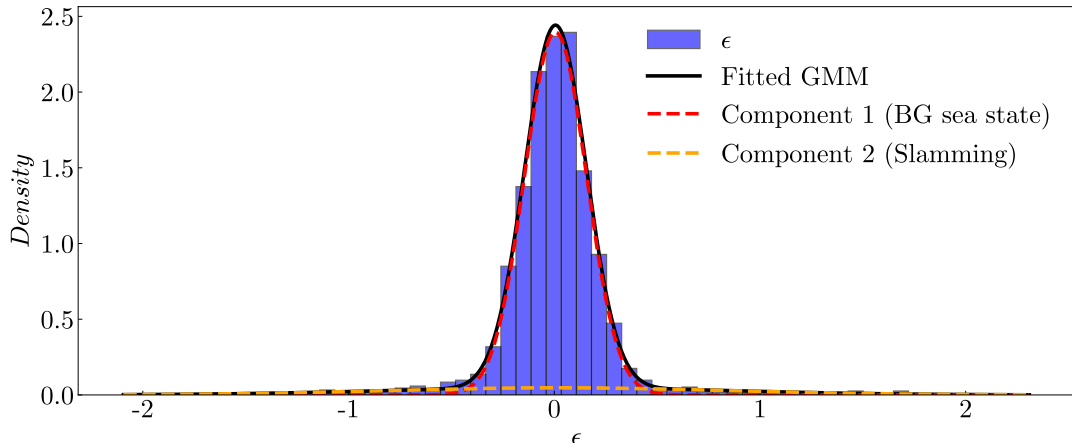


Figure 14: Distribution of two components of the 1D GMM along with the total fit.

~ 0.1 , while background sea state has a smaller variance with the probability of ~ 0.9 .

- As mentioned in the previous part, *Legendre* polynomial was chosen to account for the smooth and steadily varying trend in acceleration signal. *Legendre* polynomial was particularly chosen instead of monomial basis because of its orthogonal property within $[-1, 1]$, which helps to improve the condition number of the system.

$$\int_{-1}^1 P_i(\tilde{t})P_j(\tilde{t})d\tilde{t} = \frac{2}{2i+1}\delta_{ij}$$

For $n = 2$, the basis is

$$P_0 = 1, \quad P_1 = \tilde{t}, \quad P_2 = \frac{1}{2}(3\tilde{t}^2 - 1)$$

The harmonic basis was considered for oscillatory response of the acceleration signal. The final predictor after the regression takes the form

$$\begin{aligned} \hat{y}(t) = & -0.00744026 + 1.17051422t - 0.46714436 \cdot \frac{1}{2}(3\tilde{t}^2 - 1) - 0.05609375\cos(\pi\tilde{t}) \\ & - 0.07363466\sin(\pi\tilde{t}) + 0.0089983\cos(2\pi\tilde{t}) + 0.00805816\sin(2\pi\tilde{t}) \end{aligned} \quad (4)$$

To achieve equation (4), regularization was done using a penalization term $\lambda\Gamma^T\Gamma$ to give the system better stability by decreasing its condition number. Penalization matrix $\Gamma = \text{diag}(0, 10^{-3}, 10^{-3}, 1, 1, 4, 4)$ was chosen in such a way that the oscillatory high frequency coefficients in the equation (1) get penalization weights equal to ω_j^2 , while the low frequency coefficients get very less regularized. Optimal hyper-parameter λ was found by grid-searching over $[10^{-6}, 10^2]$ so that test *MSE* ($\lambda = 0.5541$) was minimized. This process of finding predictor is called *Ridge* regression.

The residuals $\epsilon_i = y_i - \hat{y}_i$ were modeled by a two-component 1D Gaussian Mixture Model (GMM) shown in equation (3). `sklearn.mixture.GaussianMixture` from the `scikit-learn` was used to find the weight, mean and variance of the two components. The fitted weights $(\pi_1, \pi_2) = (0.9017, 0.0983)$ and variances $(\sigma_1^2, \sigma_2^2) = (0.0226, 0.6882)$ separated the signal into two components - dominant low variance background sea and low-probability high variance slamming events, which make the noise model a good interpreter of the sea state.

A. Challenge submission I: Using the predictive model

Predicted *Vibration Dose Value* (VDV) = 1.1563152.

B. Challenge submission II: Using the GMM model

$\sigma_{bg,pred} = 0.15019996$.

```

1 import numpy as np
2 from numpy.polynomial.legendre import legvander
3 import matplotlib.pyplot as plt
4 import matplotlib as mpl
5 from numpy.linalg import solve
6 from sklearn.mixture import GaussianMixture
7 from scipy.integrate import simpson
8
9 # Load and shuffle data
10 data = np.loadtxt("hw4_train.csv", delimiter=",")
11 t = data[:, 0]
12 y = data[:, 1]
13
14 # normalize time to [-1, 1]
15 t_norm = 2 * (t - np.min(t)) / (np.max(t) - np.min(t)) - 1
16
17 # sort by time
18 id = np.argsort(t_norm)
19 t_norm = t_norm[id]
20 y = y[id]
21
22 # Use early time as training, later as validation
23 split = int(0.7 * len(t_norm))
24 t_train, y_train = t_norm[:split], y[:split]
25 t_test, y_test = t_norm[split:], y[split:]
26
27 # ===== Ridge regression model =====
28
29 # construct design matrix
30 def design_matrix(t, n_poly=2, omega=None):
31     t = np.asarray(t, dtype=float)
32     if omega is None:
33         omega = [1.0, 2.0, 3.0]
34
35     cols = []
36
37     # orthogonal polynomial trend (Legendre basis)
38     trend = legvander(t, n_poly)
39     for i in range(trend.shape[1]):
40         cols.append(trend[:, i])
41
42     # harmonic oscillations
43     for w in omega:
44         cols.append(np.cos(w * np.pi * t))
45         cols.append(np.sin(w * np.pi * t))
46
47     return np.column_stack(cols)
48
49 # train and test design matrix
50 A_train = design_matrix(t_train, n_poly=2, omega=[1.0, 2.0])
51 A_test = design_matrix(t_test, n_poly=2, omega=[1.0, 2.0])
52
53 print("\nCondition no. of  $A^T A$  (train):", np.linalg.cond(A_train.T @ A_train))
54 print("\nCondition no. of  $A^T A$  (test):", np.linalg.cond(A_test.T @ A_test))
55
56
57 # regularization function
58 def gamma_t_gamma(n_poly, omega):

```

```

59
60     weights = []
61     # polynomial terms lightly penalized
62     for i in range(n_poly + 1):
63         if i == 0:
64             weights.append(0.0)
65         else:
66             weights.append(1e-3)
67     # harmonics penalized proportionally to the square of frequency
68     for k, w in enumerate(omega, start=1):
69         strength = (k**2)
70         weights += [strength, strength]
71     return np.diag(weights)
72
73 # ridge regression function
74 def ridge_regression(A, y, Gamma_t_Gamma, lam=1e-3, trim=0.02):
75     # initial fit
76     omega = solve(A.T @ A + lam * Gamma_t_Gamma, A.T @ y)
77     y_pred = A @ omega
78     resid = y - y_pred
79
80     # trim extreme residuals (slamming)
81     if trim > 0:
82         threshold = np.quantile(np.abs(resid), 1 - trim)
83         mask = np.abs(resid) < threshold
84         A_trim, y_trim = A[mask], y[mask]
85         omega = solve(A_trim.T @ A_trim + lam * Gamma_t_Gamma, A_trim.T @ y_trim)
86
87     return omega
88
89 Gamma_t_Gamma = gamma_t_gamma(n_poly=2, omega=[1.0, 2.0])
90
91 # grid search for best fit
92 lambda_ = np.logspace(-6, 2, 40)
93 mse_train, mse_test = [], []
94 cond_train, cond_test = [], []
95
96 for lam in lambda_:
97     theta = ridge_regression(A_train, y_train, Gamma_t_Gamma, lam=lam, trim=0.02)
98     y_train_pred = A_train @ theta
99     y_test_pred = A_test @ theta
100     mse_train.append(np.mean((y_train_pred - y_train)**2))
101     mse_test.append(np.mean((y_test_pred - y_test)**2))
102
103     # regularized condition no.
104     cond_train.append(np.linalg.cond(A_train.T @ A_train + lam * Gamma_t_Gamma))
105     cond_test.append(np.linalg.cond(A_test.T @ A_test + lam * Gamma_t_Gamma))
106
107 best_id = np.argmin(mse_test)
108 lambda_best = lambda_[best_id]
109 print(f"\nBest  $\lambda = \{lambda\_best:.4e\}$ , Test MSE =  $\{mse\_test[best\_id]:.8f\}$ ")
110
111 # parameters for plotting
112 plt.rcParams["font.family"] = "serif"
113 plt.rcParams["font.serif"] = ["CMU Serif"]
114 plt.rcParams["mathtext.fontset"] = "cm"
115 plt.rcParams["font.size"] = 22
116 mpl.rcParams["axes.unicode_minus"] = False
117

```

```

118 # condition number plot
119 fig, ax = plt.subplots(figsize=(15, 6))
120 ax.loglog(lambda_, cond_train, "bo-", ms=10, lw=3, label=fr"Train $\kappa(A^T A + \lambda \Gamma^T \Gamma)$")
121 ax.loglog(lambda_, cond_test, "ro-", ms=10, lw=3, label=fr"Test $\kappa(A^T A + \lambda \Gamma^T \Gamma)$")
122 ax.axvline(lambda_best, color="k", lw=3, ls="--", label=fr"Best $\lambda = \{ \lambda_{best} : .4f \}$")
123 plt.xlabel(r"$\lambda$")
124 plt.ylabel(r"$\kappa(A^T A + \lambda \Gamma^T \Gamma)$")
125 plt.ylim(1e0, 1e11)
126 ax.legend(frameon=False, loc='best')
127 ax.tick_params(axis="both", which="both", direction="in")
128 plt.savefig("marine_cond.pdf", dpi=1080)
129 plt.show()
130
131 # mse plot
132 fig, ax = plt.subplots(figsize=(15, 6))
133 ax.loglog(lambda_, mse_train, "bo-", ms=10, lw=3, label="Train $MSE$")
134 ax.loglog(lambda_, mse_test, "ro-", ms=10, lw=3, label=r"Test $MSE$")
135 ax.axvline(lambda_best, color="k", lw=3, ls="--", label=rf"Best $\lambda = \{ \lambda_{best} : .4f \}$")
136 plt.xlabel("$\lambda$")
137 plt.ylabel("$MSE$")
138 plt.legend(frameon=False, loc="best")
139 plt.tick_params(axis="both", which="both", direction="in")
140 plt.savefig("marine_mse.pdf", dpi=1080)
141 plt.show()
142
143 # best fit model
144 theta_best = ridge_regression(A_train, y_train, Gamma_t_Gamma, lam=lambda_best,
145                               trim=0.02)
146 print("\nBest $\theta$ =", theta_best)
147
148 y_pred_train = A_train @ theta_best
149 y_pred_test = A_test @ theta_best
150 print("\nPredicted acceleration (train): \n", y_pred_train)
151 print("\nPredicted acceleration (test): \n", y_pred_test)
152
153 # de-normalize time
154 t_o = 0.5 * (t_norm + 1) * (np.max(t) - np.min(t)) + np.min(t)
155 t_train_o = t_o[:split]
156 t_test_o = t_o[split:]
157
158 # prediction plot
159 fig, ax = plt.subplots(figsize=(15, 6))
160 ax.plot(t_train_o, y_train, "bo", alpha=0.5, label="Training data")
161 ax.plot(t_test_o, y_test, "ro", alpha=0.5, label="Testing data")
162 ax.plot(t_train_o, y_pred_train, color="orange", ls="-", lw=3, label="Fit (train)"
163        )
164 ax.plot(t_test_o, y_pred_test, "k-", lw=3, label='Fit (test)')
165 plt.xlabel("$t$")
166 plt.ylabel("$y$")
167 plt.ylim(-3, 4)
168 plt.legend(frameon=False, loc="best", ncol=2)
169 plt.tick_params(axis="both", which="both", direction="in")
170 plt.savefig("marine_predict.pdf", dpi=1080)
171 plt.show()

```

```

171 # ===== GMM noise model =====
172
173 # residuals
174 resid_train = y_train - y_pred_train
175 resid_test  = y_test  - y_pred_test
176
177 # residual plot
178 fig, ax = plt.subplots(figsize=(15, 6))
179 ax.hist(resid_train, bins=60, density=True, color="blue", edgecolor="black", alpha
180         =0.6)
181 plt.xlabel(r"$\epsilon$")
182 plt.ylabel(r"$Density$")
183 plt.tick_params(axis="both", which="both", direction="in")
184 plt.savefig("marine_residual.pdf", dpi=1080)
185 plt.show()
186
187 # 1D GMM with 2 components
188 gmm = GaussianMixture(n_components=2, covariance_type="full", random_state=23)
189 gmm.fit(resid_train.reshape(-1, 1))
190
191 means = gmm.means_.ravel()
192 vars_ = gmm.covariances_.ravel()
193 stds = np.sqrt(gmm.covariances_).ravel()
194 weights = gmm.weights_.ravel()
195
196 print("\nGMM parameters using training residual")
197 for i, (w, m, v, s) in enumerate(zip(weights, means, vars_, stds)):
198     print(f"\nComponent {i+1}: weight={w:.4f}, mean={m:.4f}, variance={v:.4f}, std
199           ={s:.4f}")
200
201 # GMM plot
202 x_grid = np.linspace(min(resid_train), max(resid_train), 600).reshape(-1, 1)
203 pdf_total = np.exp(gmm.score_samples(x_grid))
204
205 # PDF of individual component
206 pdf_components = np.array([
207     w * (1 / (np.sqrt(2*np.pi) * s)) * np.exp(-0.5 * ((x_grid - m) / s)**2)
208     for w, m, s in zip(weights, means, stds)
209 ])
210
211 colors = ["red", "orange"]
212 labels = ["BG sea state", "Slamming"]
213 fig, ax = plt.subplots(figsize=(15, 6))
214 ax.hist(resid_train, bins=60, density=True, color="blue", edgecolor="black", alpha
215         =0.6, label="$\epsilon$")
216 ax.plot(x_grid, pdf_total, "k-", lw=3, label="Fitted GMM")
217 for k, (pdf, c, lbl) in enumerate(zip(pdf_components, colors, labels)):
218     ax.plot(x_grid, pdf, "--", lw=3, color=c, label=f"Component {k+1} ({lbl})")
219 plt.xlabel(r"$\epsilon$")
220 plt.ylabel(r"$Density$")
221 plt.tick_params(axis="both", which="both", direction="in")
222 plt.legend(frameon=False, loc="best")
223 plt.savefig("marine_gmm.pdf", dpi=1080)
224 plt.show()
225
226 # ===== Challenge Submission I =====
227
228 # acceleration^4
229 a4 = np.abs(y_pred_test)**4

```

```

227
228 # Trapezoidal rule
229 vdv_trap = (np.trapz(a4, t_test_o)) ** 0.25
230
231 # Simpson's rule
232 vdv_simp = (simpson(a4, t_test_o)) ** 0.25
233
234 print("\nVibration Dose Value (VDV):")
235 print(f"\nTrapezoidal rule: {vdv_trap:.8f}")
236 print(f"\nSimpsons 1/3rd rule : {vdv_simp:.8f}")
237
238 # ===== Challenge Submission II =====
239
240 id_bgc = np.argmin(stds)
241 sigma_bgc_pred = stds[id_bgc]
242 id_slm = np.argmax(stds)
243
244 sigma_ratio = stds[id_slm] / stds[id_bgc]
245 p_slam = weights[id_slm]
246
247 print("\nGMM Noise:")
248 print(f"\nBackground sea state standard deviation = {sigma_bgc_pred:.8f}")
249 print(f"\nSlamming standard deviation = {stds[id_slm]:.8f}")
250 print(f"\nRatio of standard deviation of slamming and background sea = {
    sigma_ratio:.8f}")
251 print(f"\nSlamming probability = {p_slam:.4f}")

```

Listing 5: *marine.py*


```

1 Condition no. of $A^{TA}$ (train): 110063.1089055772
2
3 Condition no. of $A^{TA}$ (test): 28642884212.86928
4
5 Best $\lambda$ = 5.5410e-01, Test MSE = 0.08193715
6
7 Best $\theta$ = [-0.00744026  1.17051422 -0.46714436 -0.05609375 -0.07363466
8               0.0089983
9               0.00805816]
10
11 Predicted acceleration (train):
12 [-1.58000678 -1.57810406 -1.57620236 ...  0.49134531  0.49176704
13        0.49218858]
14
15 GMM parameters using training residual
16
17 Component 1: weight=0.9017, mean=0.0061, variance=0.0226, std=0.1502
18
19 Component 2: weight=0.0983, mean=0.0153, variance=0.6882, std=0.8296
20
21 Vibration Dose Value (VDV):
22
23 Trapezoidal rule: 1.15631521
24
25 Simpsons 1/3rd rule : 1.15631523
26
27 GMM Noise:
28
29 Background sea state standard deviation = 0.15019996
30
31 Slamming standard deviation = 0.82955471
32
33 Ratio of standard deviation of slamming and background sea = 5.52300217
34
35 Slamming probability = 0.0983

```

Listing 6: Output terminal (selected) for *marine.py*