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References (if any):

- This assignment has to be completed in teams of two. Collaborations outside the team are strictly prohibited.
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1. (15 points) [DENSITY ESTIMATION]

- (a) (5 points) [PARAMETRIC MLE] Suppose that the lifetime of Philips brand light bulbs is modeled by an exponential distribution with (unknown) rate parameter λ or alternatively mean parameter μ . We test 6 bulbs and find they have lifetimes of 2, 6, 7, 1, 4, and 3 years, respectively. (i) (2 points) What is the MLE for λ and for μ , and (ii) (2 points) derive the bias of each of these estimators? (iii) (1 point) If the estimators are biased, how will you correct them to get unbiased estimators?

Solution:

This is MLE of λ | μ of exponential distribution $\lambda e^{-\lambda x}$

$$\begin{aligned}
 \lambda_{ml} &= \operatorname{argmax}_{\lambda} \prod_{i=1}^n P(x_i; \lambda) \\
 &= \operatorname{argmax}_{\lambda} \prod_{i=1}^n \lambda e^{-\lambda x_i} \\
 &= \operatorname{argmax}_{\lambda} \sum_{i=1}^n (\log \lambda - \lambda x_i) \\
 &= \operatorname{argmax}_{\lambda} (n \log \lambda - \lambda \sum_{i=1}^n x_i)
 \end{aligned}$$

Differentiating this expression with respect to λ we get,

$$\begin{aligned}
 \frac{n}{\lambda} - \sum_{i=1}^n x_i &= 0 \\
 \lambda &= \frac{n}{\sum_{i=1}^n x_i}, \mu_{ml} = \frac{1}{\lambda_{ml}} = \frac{\sum_{i=1}^n x_i}{n}
 \end{aligned}$$

(b) (5 points) [PARAMETRIC BAYESIAN] Assume we have following prior distribution on θ :

$$p(\theta) = \alpha \beta^\alpha \theta^{-\alpha-1} \mathbb{1}_{(\beta, \infty)}(\theta)$$

where $\mathbb{1}_{(\beta, \infty)}(\theta)$ is an indicator function which equals 1 when $\beta < \theta < \infty$ and 0 otherwise. $p(\theta)$ is called Pareto distribution which is denoted as $\theta \sim \text{Pareto}(\alpha, \beta)$.

- i. (1½ points) Assume $\theta \sim \text{Pareto}(\alpha, \beta)$ and $X_1, \dots, X_n \sim \text{Uniform}(0, \theta)$ which are conditionally independent given θ . What is the posterior distribution $p(\theta|D)$ where $D = (x_1, x_2, \dots, x_n)$. Does it belong to any family of distributions that you recognize?

Solution:

$$p(\theta) = \begin{cases} 0 & \theta \leq \beta \\ \alpha \beta^\alpha \theta^{-\alpha-1} & \beta < \theta < \infty \end{cases}$$

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)}$$

Now, $\tilde{\beta} = \max(x_1, x_2 \dots x_n)$

$$\begin{aligned} &= \frac{\frac{1}{\theta^n} \alpha \beta^{-\alpha-1}}{\int_{\tilde{\beta}}^{\infty} \frac{\alpha \beta^{\alpha} \theta^{-\alpha-1}}{\theta^n} d\theta} = \frac{\theta^{-\alpha-n-1}}{\int_{\tilde{\beta}}^{\infty} \theta^{-\alpha-n-1} d\theta} \\ &\int_{\tilde{\beta}}^{\infty} \theta^{-\alpha-n-1} d\theta = \frac{\tilde{\beta}^{-\alpha-n}}{\alpha+n} \\ \frac{\theta^{-\alpha-n-1}}{\int_{\tilde{\beta}}^{\infty} \theta^{-\alpha-n-1} d\theta} &= \frac{-\theta^{-\alpha-n} \times (\alpha+n)}{\tilde{\beta}^{-\alpha-n}} \\ &= (\alpha+n) \tilde{\beta}^{\alpha+n} \theta^{-(\alpha+n)-1} \\ &= \text{pareto}(\alpha+n, \tilde{\beta}) \end{aligned}$$

- ii. (1½ points) Using the above derived posterior, calculate the MAP estimate of θ ? How does this compare to the MLE?

Solution:

The likelihood is :

$$P(D; \theta) = \frac{1}{\theta^n}$$

MLE estimate would be $\theta = \max(x_1, x_2, x_3, \dots x_n)$ The pareto function is a strictly decreasing function from $\theta \geq \tilde{\beta}$, therefore the MAP estimate of this would be $\tilde{\beta}$.

Therefore both the MLE estimate and MAP estimate of θ would be the same.

- iii. (2 points) Square loss is defined as $L(\theta, \hat{\theta}) = (\theta - \hat{\theta})^2$. For the above derived posterior in (i), what estimator of θ minimizes the posterior expected square loss? Simplify your answer as much as possible. Is it the same as the MLE and/or the MAP?

Solution:

To minimize $L(\theta, \hat{\theta}) = (\theta - \hat{\theta})^2$ we have to minimize $E[(\theta - \hat{\theta})^2]$

$$\int_{-\infty}^{\infty} (\theta - \hat{\theta})^2 p(\theta) d\theta$$

$$\int_{-\infty}^{\infty} \theta^2 p(\theta) d\theta - 2 \int_{-\infty}^{\infty} \theta \hat{\theta} p(\theta) d\theta + \int_{-\infty}^{\infty} \hat{\theta}^2 p(\theta) d\theta$$

$$\int_{-\infty}^{\infty} \theta^2 p(\theta) d\theta - 2\hat{\theta}E[\theta] + \hat{\theta}^2 p(\theta)$$

Now differentiating by $\hat{\theta}$ we get,

$$2\hat{\theta} = 2E[\theta]$$

$$\hat{\theta} = E[\theta]$$

This function would reach its minimum value when θ takes the value $E[\theta]$. Expectation of θ is as follows:

$$\begin{aligned} E(\theta) &= \int_{\beta}^{\infty} \theta \alpha \beta^{\alpha} \theta^{-\alpha-1} d\theta \\ &= \alpha \beta^{\alpha} \int_{\beta}^{\infty} \theta^{-\alpha} d\theta \\ &= \alpha \beta^{\alpha} \left[\frac{\theta^{-\alpha+1}}{-\alpha+1} \right]_{\beta}^{\infty} \end{aligned}$$

Which is equal to,

$$E[\theta] = \begin{cases} \infty & \alpha \leq 1 \\ \frac{\alpha \beta}{\alpha-1} & \alpha > 1 \end{cases}$$

Therefore $\hat{\theta}$ is equal to,

$$\hat{\theta} = \begin{cases} \infty & \alpha \leq 1 \\ \frac{\alpha \beta}{\alpha-1} & \alpha > 1 \end{cases}$$

- (c) (5 points) [NON-PARAMETRIC METHOD] In class, we saw a Parzen window estimator using an unit hypercube as the Parzen window or kernel function; we will use an exponential kernel function here:

$$k(u) = \begin{cases} e^{-u} & u > 0, \\ 0 & u \leq 0. \end{cases}$$

If $D = \{x_1, x_2, \dots, x_n\}$ is a dataset of i.i.d. samples, each drawn from $U(0, 1)$, then (i) (3 points)

show that the mean of the estimated density $p(x)$ is given by:

$$E_D[p(x)] = \begin{cases} 0 & x < 0 \\ 1 - e^{-\frac{x}{h}} & 0 \leq x \leq 1 \\ e^{\frac{1-x}{h}} - e^{-\frac{x}{h}} & x \geq 1. \end{cases}$$

(ii) (2 points) Also, plot $E_D[p(x)]$ vs x for different values of h ($h = 1, 0.25$, and 0.0625). What do you observe?

Solution:

2. (10 points) [BAYESIAN DECISION THEORY]

(a) (5 points) [Optimal Classifier by Pen/Paper] Let L be the loss matrix defined by $L = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 0 \end{bmatrix}$,

where L_{ij} indicates the loss for an input x with i being the true class and j the predicted class. Given the data:

x	-2.9	1.4	0.4	-0.3	-0.7	0.9	1.8	0.8	-2.4	-1.4	1.2	2.3	2.8	-3.4
y	1	3	2	2	1	3	3	2	1	1	2	3	3	1

find the optimal Bayes classifier $h(x)$, and provide its decision boundaries/regions.

Solution:

$$P_{X|Y=1} = N(\mu_1, I), P(Y = 1) = \phi_1$$

$$P_{X|Y=2} = N(\mu_2, I), P(Y = 2) = \phi_2$$

$$P_{X|Y=3} = N(\mu_3, I), P(Y = 3) = \phi_3$$

Now through MLE estimation

$$\operatorname{argmax}_{\mu_1, \mu_2, \mu_3, \phi_1, \phi_2, \phi_3} \prod_{i=1}^n P(x_i | y_i) p(y_i)$$

Solving this problem we would get,

$$\mu_i = \frac{\sum_{j=1}^n x_j \mathbb{1}_{y_j = i}}{\sum_{j=1}^n \mathbb{1}_{y_j = i}} \phi_i = \frac{\sum_{i=1}^n \mathbb{1}_{y_j = i}}{n} \sigma_i = \frac{\sum_{j=1}^n (x_j - \mu_j)^2 \mathbb{1}_{y_j = i}}{\sum_{j=1}^n \mathbb{1}_{y_j = i}}$$

$$\mu_1 = \frac{-2.9 - 0.7 - 2.4 - 1.4 - 3.4}{5} = -2.16$$

$$\mu_2 = \frac{0.4 + 0.3 - 0.3 + 1.2}{4} = 0.525$$

$$\mu_3 = \frac{1.4 + 0.9 + 0.8 + 2.3 + 2.8}{5} = 7.8 \phi_1 = \frac{5}{14} \phi_2 = \frac{4}{14} \phi_3 = \frac{5}{14}$$

- (b) (5 points) Consider the problem of classifying a pattern x into one of the k classes $c = 1, 2, \dots, k$. Assume that we have two different tests to determine the class to be assigned to pattern x . Test 1 assigns x to the class that maximizes the posterior probability, whereas test 2 to a class chosen based on randomized decision rule.

Test 1: $H_1(x) = c^* = \operatorname{argmax}_c p(c|x)$

Test 2: $H_2(x) = c \sim p(c|x)$, where c is chosen based on the distribution

$P(c = i|x)$ in a random fashion.

- i. (1 point) Calculate the risk R_1 associated with test 1 in terms of the posterior probability using the zero-one loss function.

Solution:

$$\text{Loss}(c_1, c_2) = \begin{cases} 0 & c_1 = c_2 \\ 1 & c_1 \neq c_2 \end{cases}$$

$$R_1 = E[L(c, c^*)] = \sum_{c \sim p(c|x)}^k L(c, c^*) p = 1 - p(c^*|x)$$

- ii. (2 points) Calculate the risk R_2 associated with test 2 in terms of the posterior probability using the zero-one loss function.

Solution:

$$\begin{aligned}
 \text{Loss}(c_1, c_2) &= \begin{cases} 0 & c_1 = c_2 \\ 1 & c_1 \neq c_2 \end{cases} \\
 R_1 = \mathbb{E}_{c \sim p(c|x), c^* \sim p(c^*|x)}[L(c, c^*)] &= \sum_{j=1}^k \sum_{i=1}^k L(i, j) p(c = i|x) p(c^* = j|x) \\
 &= \sum_{j=1}^k (1 - p(c^* = j|x)) p(c^* = j|x) \\
 &= \sum_{j=1}^k p(c^* = j|x) - \sum_{i=1}^k (p(c^* = j|x))^2 \\
 &= 1 - \sum_{j=1}^k (p(c^* = j|x))^2
 \end{aligned}$$

- iii. (2 points) Which test do you think would perform better always based on the risks R_1 and R_2 ? Also, specify the conditions under which both the tests behave the same.

Solution:

R_1 is better than R_2

$$R_1 = R_2 \text{ if } P(c^*|x) = 1 \text{ and all other } P(c_i|x) = 0$$

3. (15 points) [Linear regression]

- (a) (5 points) Say we have a linear regression dataset where every training datapoint $\{x_n, y_n\}$ has a weight q_n ($q_n > 0$) identified with it. Then we have the weighted error function (sum of squares) given by:

$$E_q(w) = \sum_{n=1}^N \frac{q_n (t_n - w^T x_n)^2}{2}.$$

Derive the closed form solution for the minimizer w^* of this function. Express it in matrix format for a simplified expression.

Solution:

$$E_q(w) = \sum_{n=1}^N \frac{((q_n)^{1/2} t_n - (q_n)^{1/2} w^T x_n)^2}{2}$$

$$\mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_N \end{bmatrix} \quad \mathbf{t}_q = \begin{bmatrix} t_1(q_1)^{1/2} \\ t_2(q_2)^{1/2} \\ \vdots \\ t_N(q_N)^{1/2} \end{bmatrix}$$

$$\mathbf{x}_n = \begin{bmatrix} x_n^{(1)} \\ x_n^{(2)} \\ \vdots \\ x_n^{(D)} \end{bmatrix} \quad \mathbf{x}_{nq} = \begin{bmatrix} x_n^{(1)}(q_n^{(1)})^{1/2} \\ x_n^{(2)}(q_n^{(2)})^{1/2} \\ \vdots \\ x_n^{(D)}(q_n^{(D)})^{1/2} \end{bmatrix}$$

$$\mathbf{X}_q = \begin{bmatrix} x_{1q} \\ x_{2q} \\ \vdots \\ x_{Nq} \end{bmatrix}$$

$$\sum_{n=1}^N (t_n - \mathbf{w}^T \mathbf{x}_{nq})$$

This equation is similar to the equation,

$$\sum_{n=1}^N (t_n - \mathbf{w}^T \mathbf{x}_n)$$

The \mathbf{w} which minimizes the above equation is,

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{t}$$

Similarly the \mathbf{w} which will minimize

$$\sum_{n=1}^N (t_n - \mathbf{w}^T \mathbf{x}_{nq})$$

$$\mathbf{w}^* = (\mathbf{X}_q^T \mathbf{X}_q)^{-1} \mathbf{X}_q^T \mathbf{t}_q$$

(b) (5 points) We saw in class that the error function in case of ridge regression is given by:

$$\tilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N (t_n - \mathbf{w}^T \phi(\mathbf{x}_n))^2 + \frac{\lambda}{2} \mathbf{w}^T \mathbf{w}.$$

Show that this error function is convex and is minimized by:

$$\mathbf{w}^* = (\lambda \mathbf{I} + \phi^T \phi)^{-1} \phi^T \mathbf{t}.$$

Also show that $(\lambda I + \phi^T \phi)$ is invertible for any $\lambda > 0$.

Solution:

We know that in this expression the first term on the RHS is convex, the second term on RHS is also convex as it is $\|x\|^2$.

$$\tilde{E}(w) = \frac{1}{2} \sum_{n=1}^N (t_n - w^T \phi(x_n))^2 + \frac{\lambda}{2} w^T w.$$

As we know that sum of two convex functions is convex $\tilde{E}(w)$ is therefore convex.

Now to find w^* , take gradient and put it to zero.

$$\begin{aligned} \Phi^T \Phi w - \Phi^T t + \lambda w &= 0 \\ &= (\Phi^T \Phi + \lambda I) w = \Phi^T t \\ w &= (\Phi^T \Phi + \lambda I)^{-1} \Phi^T t \end{aligned}$$

TP : $(\lambda I + \phi^T \phi)$ is invertible for any $\lambda > 0$

Proof by contradiction: Assume that $|\lambda I + \phi^T \phi| = 0$ and $\lambda > 0$. $\phi^T \phi$ is PSD, so all the eigen values of this are positive.

Suppose say that $|\lambda I + \phi^T \phi| = 0$. That would mean that $-\lambda$ is an eigen value of the $\phi^T \phi$. As we have assumed that λ is positive therefore $-\lambda$ is negative and therefore $\phi^T \phi$ has a negative eigen value which is not possible, therefore by contradiction we have proved that $(\lambda I + \phi^T \phi)$ is invertible for any $\lambda > 0$

(c) (5 points) Given a dataset

$$X = \begin{bmatrix} -2 & 6 \\ -1 & 3 \end{bmatrix} \quad t = \begin{bmatrix} 3 \\ -1 \end{bmatrix}$$

find all minimizers w of $E(w) = \frac{1}{2} \|Xw - t\|^2$, and indicate the one with the smallest norm. How does your answer change if you are looking for minimizers of $\tilde{E}(w)$ instead (assuming $\lambda = 1$)?

Solution:

$$E(w) = \frac{1}{2} ((-2w_1 + 6w_2 - 3)^2 + (-w_1 + 3w_2 + 1)^2)$$

Differentiating this wrt w_1 we get,

$$w_1 - 3w_2 + 1 = 0$$

Differentiating this wrt w_2 we get,

$$w_1 - 3w_2 + 1 = 0 \quad (1)$$

To find the one with the smallest norm we have to minimize $w_1^2 + w_2^2$. Substituting (1) in this we get,

$$w_1^2 + \left(\frac{w_1 + 1}{3}\right)^2$$

Differentiating this and equating to zero and solving for w_1 we get,

$$w_1 = \frac{-1}{10}, w_2 = \frac{3}{10}$$

Now, to find the value of w when $\lambda = 1$ we have the equation.

$$w = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T t$$

In this case Φ is same as X therefore,

$$w = (X^T X + I)^{-1} X^T t$$

Substituting X and t in this we would get,

$$w = \begin{bmatrix} -1/4 \\ 1/4 \end{bmatrix}$$

4. (5 points) [Kernel methods] Let K_1, K_2 be two arbitrary valid kernel functions mapping vectors from $\mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$. For each of the cases below, show if it is a valid kernel or not with supporting arguments. (Hint: Keep your solutions brief by using earlier parts of this question to solve later parts whenever possible.)

- (a) (1 point) $K_3(x, y) = K_1(x, y) + K_2(x, y) + 7.5$

Solution: As K_1 and K_2 are PSD, Therefore is also PSD,

$$\begin{aligned} x(K_1 + K_2 + 7.5I)x^T \\ = x(K_1)x^T + x(K_2)x^T + xx^T \end{aligned}$$

which is PSD as first and second terms are positive as they are kernels and the third term is the second norm which is positive.

(b) (1 point) $K_4(x, y) = K_1(x, y)K_2(x, y)$ (product of two kernels)

Solution:

$$\begin{aligned}
 k_1(x, y) &= \sum_{i=1}^n \Phi_i^1 \Phi_i^1(y) \\
 k_2(x, y) &= \sum_{j=1}^n \Phi_j^2 \Phi_j^2(y) \\
 k_1(x, y)k_2(x, y) &= \sum_{i,j} \Phi_i^1 \Phi_i^1(y) \Phi_j^2 \Phi_j^2(y) \\
 &= \sum_k \Phi_k^3(x) \Phi_k^y \\
 k_4 &= \sum_k \Phi_k^3(x) \Phi_k^y
 \end{aligned}$$

Therefore, it is set of finite basis basics, which would also be a kernel.

(c) (1 point) $K_5(x, y) = (x^T y + 1)^{73}$

Solution:

$$\begin{aligned}
 K_5(x, y) &= (1 + z)^n = \sum_{k=1}^n \binom{n}{k} x^k \\
 &= \sum_{k=1}^{73} \binom{73}{k} (x^T y)^k \\
 &= \sum_{k=1}^n K_k(x, y)
 \end{aligned}$$

We know sum of kernels is kernel using first part of the question.

(d) (1 point) $K_6(x, y) = 6K_1(x, y) - 3K_2(x, y)$

Solution: $K_6(x, y)$ is not a kernel function. Proof by counter example :

Let $K_1(x, y) = K(x, y)$ and $K_2(x, y) = 3k(x, y)$ be valid kernels then $K_6(x, y) = 6k(x, y) - 9k(x, y) = -3k(x, y)$ which is not a kernel matrix as it is not positive semi definite.

$$x(6K_1 - 3K_2)x^T = -3x^T k(x, y)x \leq 0$$

(e) (1 point) $K(x, y) = \exp(2x^T y)$ (Hint: Consider polynomial expansion of $\exp(t)$.)

Solution:

$$z^T \exp(2u^T v) z \exp(2u^T v) = 2(1 + uv + (u^T v)^2 \dots)$$

Each expression is a kernel.

Therefore this expression is of the form,

$$z^T k_1 z + z^T k_2 z + z^T k_1 z + z^T k_3 z \geq 0$$

the kernel is PSD, and the equation is symmetric because

5. (10 points) [LET'S ROLL UP YOUR CODING SLEEVES...] **Learning Binary Bayes Classifiers from data via Density Estimation**

Derive Bayes classifiers under assumptions below and employing maximum likelihood approach to estimate class prior/conditional densities, and return the results on a test set.

1. **BayesA** Assume $X|Y = -1 \sim \mathcal{N}(\mu_-, I)$ and $X|Y = 1 \sim \mathcal{N}(\mu_+, I)$
2. **BayesB** Assume $X|Y = -1 \sim \mathcal{N}(\mu_-, \Sigma)$ and $X|Y = 1 \sim \mathcal{N}(\mu_+, \Sigma)$
3. **BayesC** Assume $X|Y = -1 \sim \mathcal{N}(\mu_-, \Sigma_-)$ and $X|Y = 1 \sim \mathcal{N}(\mu_+, \Sigma_+)$

Please see [this folder](#) for the template .ipynb file containing the helper functions, and you've to add the missing code to this file (specifically, three functions `function_for_A`, `function_for_B`, `function_for_C` and associated plotting/ROC code snippets) to implement the above three algorithms for the 2 datasets given in the same folder.

(Note: Please provide your results/answers in the pdf file you upload to GradeScope, but submit your code separately in [this](#) moodle link. The code submitted should be a `rollno1_rollno2.zip` file containing a folder named Q5 with two files: `rollno1_rollno2.ipynb` file (including your code as well as the exact same results/plots uploaded to Gradescope) and the associated `rollno1_rollno2.py` file.)

- (a) (3 points) Plot all the classifiers (3 classification algorithms on 2 datasets = 6 plots) on a 2D plot, Add the training data points also on the plots. (Color the positively classified area light green, and negatively classified area light red as in Fig 4.5 in Bishop's book).

Solution:

- (b) (3 points) Give the ROC curves for all the classifiers. Note that a ROC curve plots the FPR (False Positive Rate) on the x-axis and TPR (True Positive Rate) on the y-axis.

Solution:

- (c) (2 points) Provide the error rates for the above classifiers (3 classifiers on the two datasets as 3×2 table, with appropriately named rows and columns).

Solution:

- (d) (2 points) Summarise and explain your observations based on your plots and the assumptions given in the problem. Also briefly comment whether a non-parametric density estimation approach could have been used to solve this problem, and if so, what the associated pros/cons are compared to the parametric MLE based approach you have implemented.

Solution:

6. (5 points) [CODING A DIFFERENT DENSITY ESTIMATION?] In the previous question, the class conditional densities were Gaussian. But not all real-world datasets are Gaussian as is to begin with. For instance, consider this data on expression/activity level of genes in the skeletal muscle tissue of different individuals, provided as a “Genes \times Samples” matrix in this [link](#). (Note: Put all your code pertaining to this question into a single file `rollno1_rollno2_genes.<fileextension>`, and include this single file inside the Q6 folder of the `rollno1_rollno2.zip` file mentioned in the previous question.)
- (a) (2 points) (Model Selection) How would you model any given gene in this dataset, i.e., what distribution will you assume for a gene? Assume that every gene follows the same parametric model/distribution, but with different parameter values. Support your assumption.

Solution:

- (b) (2 points) (MLE Code) How will you obtain the MLE estimates of the assumed model’s parameters? (no need to derive it, just state your answer as a closed-form formula or as an optimization method). Write a code to estimate these parameters for each gene.

Solution:

- (c) (1 point) (Diagnostic Plots) Use your code to also plot the sample mean (x-axis) vs. sample variance (y-axis) of each gene (across all genes, with each dot in this scatter-plot being a gene). Overlay on this plot using a different color, the model mean vs. variance of each gene (i.e., mean/variance calculated using the expectation/variance formula implied by the model/distribution learnt via MLE). What does this plot tell you?

Solution: