10/36-702 Statistical Machine Learning Homework #2 Solutions

DUE: 3:00 PM February 22, 2019

Problem 1 [10 pts.]

Consider the data $(X_1, Y_1), \ldots, (X_n, Y_n)$ where $X_i \in \mathbb{R}$ and $Y_i \in \mathbb{R}$. Inspired by the fact that $\mathbb{E}[Y|X = x] = \int yp(x, y) dy/p(x)$, define

$$\widehat{m}(x) = \frac{\int y \widehat{p}(x, y) dy}{\widehat{p}(x)}$$

where

$$\widehat{p}(x) = \frac{1}{n} \sum_{i} \frac{1}{h} K\left(\frac{X_i - x}{h}\right)$$

and

$$\widehat{p}(x,y) = \frac{1}{n} \sum_{i} \frac{1}{h^2} K\left(\frac{X_i - x}{h}\right) K\left(\frac{Y_i - y}{h}\right).$$

Assume that $\int K(u)du = 1$ and $\int uK(u)du = 0$. Show that $\widehat{m}(x)$ is exactly the kernel regression estimator that we defined in class.

Solution.

$$\begin{aligned} \frac{\int y \cdot \widehat{p}(x,y) dy}{\widehat{p}(x)} &= \frac{\frac{1}{nh^2} \int y \sum K(\frac{x-X_i}{h}) K(\frac{y-Y_i}{h}) dy}{\frac{1}{nh} \sum K(\frac{x-X_i}{h})} \\ &= \frac{\sum K(\frac{x-X_i}{h}) \int y \frac{1}{h} K(\frac{y-Y_i}{h}) dy}{\sum K(\frac{x-X_i}{h})} \\ &= \frac{\sum K(\frac{x-X_i}{h}) Y_i}{\sum K(\frac{x-X_i}{h})} \\ &= \widehat{m}(x). \end{aligned}$$

Problem 2 [15 pts.]

Suppose that (X, Y) is bivariate Normal:

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim N\left(\begin{pmatrix} \mu \\ \eta \end{pmatrix}, \begin{pmatrix} \sigma^2 & \rho \sigma \tau \\ \rho \sigma \tau & \tau^2 \end{pmatrix}\right)$$

- (a) (5 pts.) Show that $m(x) = \mathbb{E}[Y|X = x] = \alpha + \beta x$ and find explicit expressions for α and β .
- (b) (5 pts.) Find the maximum likelihood estimator $\widehat{m}(x) = \widehat{\alpha} + \widehat{\beta}x$.
- (c) (5 pts.) Show that $|\widehat{m}(x) m(x)|^2 = O_P(n^{-1})$.

Solution.

(a) Some simple calculations show

$$Y|X = x \sim N\left(\eta + \frac{\tau}{\sigma}\rho(x-\mu), \ (1-\rho^2)\tau^2\right),$$

which gives

$$\alpha = \eta - \frac{\tau \rho \mu}{\sigma}$$
 and $\beta = \frac{\tau \rho}{\sigma}$.

(b) Given a sample $(X_1, Y_1), \ldots, (X_n, Y_n)$, the MLEs for the bivariate normal parameters are

$$\widehat{\mu} = \overline{X}$$

$$\widehat{\eta} = \overline{Y}$$

$$\widehat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \overline{X})^2$$

$$\widehat{\tau}^2 = \frac{1}{n} \sum_{i=1}^n (Y_i - \overline{Y})^2$$

$$\widehat{\operatorname{Cov}}(X, Y) = \frac{1}{n} \sum_{i=1}^n (X_i - \overline{X})(Y_i - \overline{Y}).$$

Note $\beta = \frac{\tau \rho}{\sigma} = \frac{\tau \rho \sigma}{\sigma^2}$. Then by the equivariance property of the MLE,

$$\widehat{\beta} = \frac{\widehat{\mathrm{Cov}}(X,Y)}{\widehat{\sigma}^2}$$

and

$$\widehat{\alpha} = \overline{Y} - \widehat{\beta}\overline{X}.$$

Again by equivariance,

$$\widehat{m}(x) = \widehat{\alpha} + \beta x$$

(c) $\widehat{m}(x)$ is an MLE and satisfies the regularity conditions for asymptotic normality. Therefore,

$$\sqrt{n}(\widehat{m}(x) - m(x)) \sim N(0, I^{-1}(m(x))),$$

which implies

$$\sqrt{n}|\widehat{m}(x) - m(x)| = O_p(1) \implies |\widehat{m}(x) - m(x)|^2 = O_p(n^{-1}).$$

Problem 3 [20 pts.]

Let $m(x) = \mathbb{E}[Y|X = x]$. Let $X \in [0, 1]^d$. Divide $[0, 1]^d$ into cubes B_1, \ldots, B_N whose sides have length h. The data are $(X_1, Y_1), \ldots, (X_n, Y_n)$. In this problem, treat the X_i 's as fixed. Assume that the number of observations in each bin is positive. Let

$$\widehat{m}(x) = \frac{1}{n(x)} \sum_{i} Y_{i} \mathbb{1}(X_{i} \in B(x))$$

where B(x) is the cube containing x and $n(x) = \sum_i \mathbb{1}(X_i \in B(x))$. Assume that

$$|m(y) - m(x)| \le L ||x - y||_2$$

for all x, y. You may further assume that $\sup_x \operatorname{Var}(Y|X = x) < \infty$.

(a) (10 pts.) Show that

$$|\mathbb{E}[\widehat{m}(x)] - m(x)| \le C_1 h$$

for some $C_1 > 0$. Also show that

$$\operatorname{Var}(\widehat{m}(x)) \leq \frac{C_2}{n(x)}$$

for some $C_2 > 0$.

(b) (10 pts.) Now let X be random and assume that X has a uniform density on $[0,1]^d$. Let $h \equiv h_n = (C \log n/n)^{1/d}$. Show that, for C > 0 large enough, $P(\min n_j = 0) \to 0$ as $n \to \infty$ where n_j is the number of observations in cube B_j .

Solution.

(a) We have that X_i are fixed, so that $m(X_i) = Y_i$. Were they not, the below is still applicable by using the law of iterated expectation and the law of total variance.

$$\left|\mathbb{E}[\widehat{m}(x)] - m(x)\right| = \left|\mathbb{E}\left[\frac{1}{n(x)}\sum_{i}Y_{i}\mathbb{1}_{\{X_{i}\in B(x)\}}\right] - m(x)\right|$$
$$= \left|\frac{1}{n(x)}\sum_{i}\left(\mathbb{E}[Y_{i}] - m(x)\right)\mathbb{1}_{\{X_{i}\in B(x)\}}\right|$$
$$= \left|\frac{1}{n(x)}\sum_{i}\left(m(X_{i}) - m(x)\right)\mathbb{1}_{\{X_{i}\in B(x)\}}\right|$$
$$\leq \frac{1}{n(x)}\sum_{i}\left|m(X_{i}) - m(x)\right|\mathbb{1}_{\{X_{i}\in B(x)\}}$$
$$\leq \frac{1}{n(x)}\sum_{i}L\sqrt{dh} \cdot \mathbb{1}_{\{X_{i}\in B(x)\}}$$
$$= L\sqrt{dh}$$

With the first upper bound due to triangular inequality and the second one because, given $x, y \in B_i$:

$$||x - y||_2^2 = \sum_{j=1}^d (x_j - y_j)^2 \le dh^2 \implies ||x - y||_2 \le \sqrt{d}h$$

Let $\sup_x \operatorname{Var}(Y|X = x) = M$.

$$\operatorname{Var}(\widehat{m}(x)) = \operatorname{Var}\left(\frac{1}{n(x)} \sum_{i} Y_{i} \mathbb{1}_{\{X_{i} \in B(x)\}}\right)$$
$$= \frac{1}{n^{2}(x)} \sum_{i} \operatorname{Var}(Y_{i}) \mathbb{1}_{\{X_{i} \in B(x)\}}$$
$$\leq \frac{M}{n(x)}.$$

(b)

$$P(\min_{j} n_{j} = 0) = P\left(\bigcup_{j=1}^{B} \{n_{j} = 0\}\right)$$
$$\leq \sum_{j=1}^{B} P(n_{j} = 0)$$
$$= \sum_{j=1}^{B} \prod_{i=1}^{n} (1 - P(X_{i} \in B_{j}))$$
$$= \frac{1}{h^{d}} (1 - h^{d})^{n}$$
$$= \frac{n}{C \log n} \left(1 - \frac{C \log n}{n}\right)^{n}$$

Since $B = \frac{1}{h^d} \cdot 1$ Take C = 1. Then

$$\frac{n}{C\log n} \left(1 - \frac{C\log n}{n} \right)^n < \frac{n}{C\log n} e^{-\frac{C\log n}{n} \cdot n}$$
$$= \frac{n}{C\log n} n^{-C}$$
$$= \frac{1}{C\log n}$$
$$\to 0.$$

¹ if we assume 1/h is an integer, otherwise we could use that as an upper bound.

Problem 4 [15 pts.]

Consider the RKHS problem

$$\widehat{f} = \operatorname{argmin}_{f \in \mathcal{H}} \sum_{i=1}^{n} \left(y_i - f(x_i) \right)^2 + \lambda \| f \|_{\mathcal{H}}^2, \tag{1}$$

for some Mercer kernel function $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$. In this problem, you will prove that the above problem is equivalent to the finite dimensional one

$$\widehat{\alpha} = \operatorname{argmin}_{\alpha \in \mathbb{R}^n} \| y - K\alpha \|_2^2 + \lambda \alpha^T K\alpha,$$
(2)

where $K \in \mathbb{R}^{n \times n}$ denotes the kernel matrix $K_{ij} = K(x_i, x_j)$. Recall that the functions $K(\cdot, x_i)$, i = 1, ..., n are called the *representers of evaluation*. Recall that

- $(f, K(\cdot, x_i))_{\mathcal{H}} = f(x_i)$, for any function $f \in \mathcal{H}$
- $||f||_{\mathcal{H}}^2 = \sum_{i,j=1}^n \alpha_i \alpha_j K(x_i, x_j)$ for any function $f = \sum_{i=1}^n \alpha_i K(\cdot, x_i)$.
- (a) (5 pts.) Let $f = \sum_{i=1}^{n} \alpha_i K(\cdot, x_i)$, and consider defining a function $\tilde{f} = f + \rho$, where ρ is any function orthogonal to $K(\cdot, x_i)$, i = 1, ..., n. Using the properties of the representers, prove that $\tilde{f}(x_i) = f(x_i)$ for all i = 1, ..., n, and $\|\tilde{f}\|_{\mathcal{H}}^2 \ge \|f\|_{\mathcal{H}}^2$.
- (b) (10 pts.) Conclude from part (a) that in the infinite-dimensional problem (1), we need only consider functions of the form $f = \sum_{i=1}^{n} \alpha_i K(\cdot, x_i)$, and that this in turn reduces to (2).

Solution.

(a) Since $f, \tilde{f} \in \mathcal{H}_K$, for all $i = 1, \ldots, n$

$$\widetilde{f}(x_i) = \langle \widetilde{f}, K(\cdot, x_i) \rangle_{\mathcal{H}_K} = \langle f, K(\cdot, x_i) \rangle_{\mathcal{H}_K} + \langle \rho, K(\cdot, x_i) \rangle_{\mathcal{H}_K} = \langle f, K(\cdot, x_i) \rangle_{\mathcal{H}_K} = f(x_i).$$

Also, because

$$\langle \rho, f \rangle_{\mathcal{H}_K} = \left(\rho, \sum_{i=1}^n \alpha_i K(\cdot, x_i) \right)_{\mathcal{H}_K}$$
$$= \sum_{i=1}^n \alpha_i \langle \rho, K(\cdot, x_i) \rangle_{\mathcal{H}_K}$$
$$= 0,$$

we have,

$$\begin{split} \|\widetilde{f}\|_{\mathcal{H}_{K}}^{2} &= \langle f, f \rangle_{\mathcal{H}_{K}} + \langle \rho, \rho \rangle_{\mathcal{H}_{K}} + 2 \langle \rho, f \rangle_{\mathcal{H}_{K}} \\ &= \|f\|_{\mathcal{H}_{K}}^{2} + \|\rho\|_{\mathcal{H}_{K}}^{2} \\ &\geq \|f\|_{\mathcal{H}_{K}}^{2}. \end{split}$$

(b) For any $\widetilde{f} \in \mathcal{H}_K$, let $\widetilde{y} = (\widetilde{f}(x_1), \dots, \widetilde{f}(x_n))^T \in \mathbb{R}^n$. Let $f \in \mathcal{H}_K$ be $f = \sum_{i=1}^n \alpha_i K(\cdot, x_i)$, where $\alpha = K^{-1} \widetilde{y}$. Then

$$\begin{split} \langle \widetilde{f} - f, K(\cdot, x_i) \rangle_{\mathcal{H}_K} &= \langle \widetilde{f}, K(\cdot, x_i) \rangle_{\mathcal{H}_K} - \sum_{j=1}^n \alpha_j \langle K(\cdot, x_j), K(\cdot, x_i) \rangle_{\mathcal{H}_K} \\ &= \widetilde{f}(x_i) - \sum_{j=1}^n \alpha_j K(x_i, x_j) \\ &= \widetilde{f}(x_i) - [K(K^{-1}\widetilde{y})]_i \\ &= \widetilde{f}(x_i) - \widetilde{f}(x_i) \\ &= 0. \end{split}$$

Hence, $\tilde{f} - f \perp K(\cdot, x_i)$ for all i = 1, ..., n, and from (a), this implies $\tilde{f}(x_i) = f(x_i)$ for all i = 1, ..., n, and $\|\tilde{f}\|_{\mathcal{H}_K}^2 \ge \|f\|_{\mathcal{H}_K}^2$, where equality holds if and only if $\tilde{f} = f$. Therefore,

$$\sum_{i=1}^{n} \left(y_i - f(x_i) \right)^2 + \lambda \|f\|_{\mathcal{H}_K}^2 \leq \sum_{i=1}^{n} \left(y_i - \widetilde{f}(x_i) \right)^2 + \lambda \|\widetilde{f}\|_{\mathcal{H}_K}^2,$$

where equality holds if and only if $\tilde{f} = f$. Hence if $\tilde{f} = \operatorname{argmin}_{f \in \mathcal{H}_K} \sum_{i=1}^n (y_i - f(x_i))^2 + \lambda \|f\|_{\mathcal{H}_K}^2$, then $\tilde{f} = \sum_{i=1}^n \alpha_i K(\cdot, x_i)$ with $\alpha = K^{-1} \tilde{y}$. So we only need to consider functions of the form $f = \sum_{i=1}^n \alpha_i K(\cdot, x_i)$. By plugging in, we have

$$\sum_{i=1}^{n} (y_i - f(x_i))^2 \lambda \|f\|_{\mathcal{H}_K}^2 = \sum_{i=1}^{n} \left(y_i \sum_{j=1}^{n} \alpha_j K(x_i, x_j) \right)^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j K(x_i, x_j)$$
$$= \|y - K\alpha\|_2^2 + \lambda \alpha^T K\alpha.$$

Problem 5 [15 pts.]

Let $X = (X(1), \ldots, X(d)) \in \mathbb{R}^d$ and $Y \in \mathbb{R}$. In the questions below, make any reasonable assumptions that you need but state your assumptions.

- (a) (5 pts.) Prove that $\mathbb{E}(Y m(X))^2$ is minimized by choosing $m(x) = \mathbb{E}(Y|X = x)$.
- (b) (5 pts.) Find the function m(x) that minimizes $\mathbb{E}|Y m(X)|$. (You can assume that the conditional cdf F(y|X = x) is continuous and strictly increasing, for every x.)
- (c) (5 pts.) Prove that $\mathbb{E}(Y \beta^T X)^2$ is minimized by choosing $\beta_* = B^{-1}\alpha$ where $B = \mathbb{E}(XX^T)$ and $\alpha = (\alpha_1, \dots, \alpha_d)$ and $\alpha_j = \mathbb{E}(YX(j))$.

Solution.

(a) Let g(x) be any function of x. Then

$$\mathbb{E}(Y - g(X))^{2} = \mathbb{E}(Y - m(X) + m(X) - g(X))^{2}$$

$$= \mathbb{E}(Y - m(X))^{2} + \mathbb{E}(m(X) - g(X))^{2} + 2\mathbb{E}((Y - m(X))(m(X) - g(X)))$$

$$\geq \mathbb{E}(Y - m(X))^{2} + 2\mathbb{E}((Y - m(X))(m(X) - g(X)) | X)$$

$$= \mathbb{E}(Y - m(X))^{2} + 2\mathbb{E}\left((\mathbb{E}(Y|X) - m(X))(m(X) - g(X))\right)$$

$$= \mathbb{E}(Y - m(X))^{2} + 2\mathbb{E}\left((m(X) - m(X))(m(X) - g(X))\right)$$

$$= \mathbb{E}(Y - m(X))^{2} + 2\mathbb{E}\left((m(X) - m(X))(m(X) - g(X))\right)$$

(b) Let g(x) be any function of x. Recall that

$$\mathbb{E}[|Y - g(X)|] = \mathbb{E}\{\mathbb{E}[|Y - g(X)| | X]\}$$

The idea is to choose c such that $\mathbb{E}[|Y - c| | X = x]$ is minimized. Now define:

$$r(c) = \mathbb{E}[|Y - c| \mid X = x] = \int |y - c| p_{Y|X=x}(y) dy$$

The function $h_y(c) = |y - c|$ is differentiable everywhere except when y = c. Thus for $c \neq y$

$$h'_{y}(c) = \begin{cases} 1 & c > y \\ -1 & c < y \end{cases} = \mathbb{1}(c > y) - \mathbb{1}(c < y).$$

Since Y is continuous and has a density function, P(Y = c) = 0. So to minimize r(c) we can differentiate under the integral sign and set the derivative equal to 0 to obtain:

$$\begin{aligned} r'(c) &= \int h'_{y}(c) p_{Y|X=x}(y) dy = \int_{-\infty}^{c} p_{Y|X=x}(y) dy - \int_{c}^{\infty} p_{Y|X=x}(y) dy \\ &= 2 \int_{-\infty}^{c} p_{Y|X=x}(y) dy - 1 = 0 \\ &\iff \int_{-\infty}^{c} p_{Y|X=x}(y) dy = \frac{1}{2}, \end{aligned}$$

so that c = m(x), which is the median of $p_{Y|X=x}(y)$. It is a minimum since r'(c) < 0 for c < m(x) and r'(c) > 0 for c > m(x). Since m minimizes $\mathbb{E}[|Y - c| | X = x]$ at every x for any g we get

$$\mathbb{E}[|Y - g(X)| - |Y - m(X)|| X = x] \ge 0$$

which implies

$$R(g) - R(m) = \mathbb{E}[|Y - g(X)| - |Y - m(X)|] = \mathbb{E}\{\mathbb{E}[|Y - g(X)| - Y - m(X)||X]\} \ge 0.$$

(c) By setting the first derivative of the loss function equal to 0 we obtain:

$$\frac{\partial R(\beta)}{\partial \beta} = 0$$

$$\implies \frac{\partial \mathbb{E}(Y - \beta^T X)^2}{\partial \beta} = 0$$

$$\implies \mathbb{E}\Big[-2X(Y - \beta^T X)\Big] = 0$$

$$\implies 2B\beta - 2\alpha = 0$$

$$\implies \beta_* = B^{-1}\alpha,$$

where we can exchange the derivative and expectation by the dominated convergence theorem. The loss function $R(\beta)$ is strictly convex so β_* is its unique minimum.

Problem 6 [25 pts.]

Consider the many Normal means problem where we observe $Y_i \sim N(\theta_i, 1)$ for $i = 1, \dots, d$. Let $\hat{\theta}$ minimize the penalized loss

$$\sum_{i} (Y_i - \theta_i)^2 + \lambda J(\theta).$$

Find an explicit form for $\hat{\theta}$ in three cases: (i) (10 pts.) $J(\beta) = \|\theta\|_0$, (ii) (10 pts.) $J(\beta) = \|\theta\|_1$ and (iii) (5 pts.) $J(\beta) = \|\theta\|_2^2$.

Solution.

(i) Note that

$$\sum_{i} (Y_i - \theta_i)^2 + \lambda \|\theta\|_0 = \sum_{j=1}^d \left((Y_i - \theta_i)^2 + \lambda \mathbb{1}(\theta_i \neq 0) \right)$$

Then for each term i,

$$(Y_i - \theta_i)^2 + \lambda \mathbb{1}(\theta_i \neq 0) \ge Y_i^2 \mathbb{1}(\theta_i = 0) + \lambda \mathbb{1}(\theta_i \neq 0)$$
$$\ge \min\left\{Y_i^2, \lambda\right\}$$

and equality holds if and only if

$$\widehat{\theta_i} = \begin{cases} 0 & \text{if } Y_i^2 < \lambda \\ 0 \text{ or } Y_i & \text{if } Y_i^2 = \lambda \\ Y_i & \text{if } Y_i^2 > \lambda. \end{cases}$$

Hence

$$\sum_{i} (Y_i - \theta_i)^2 + \lambda \|\theta\|_0 = \sum_{j=1}^d \left((Y_i - \theta_i)^2 + \lambda \mathbb{1}(\theta_i \neq 0) \right)$$
$$\geq \sum_{j=1}^d \min\left\{ Y_i^2, \lambda \right\}$$

and equality holds if and only if

$$\widehat{\theta_i} = \begin{cases} 0 & \text{if } |Y_i| < \sqrt{\lambda} \\ 0 \text{ or } Y_i & \text{if } |Y_i| = \sqrt{\lambda} \\ Y_i & \text{if } |Y_i| > \sqrt{\lambda} \end{cases}$$

(ii) First write

$$\min_{\theta} \sum_{i} (Y_i - \theta_i)^2 + \lambda \|\theta\|_1 = \min_{\theta} \sum_{i} \left(-2Y_i \theta_i + \theta_i^2 + \lambda |\theta_i|\right).$$

Now note it is simply equivalent to

$$\begin{split} \min_{\theta_i} -2Y_i\theta_i + \theta_i^2 + \lambda|\theta_i| \\ \iff \min_{\theta_i} -2\widehat{\theta}_i^{OLS}\theta_i + \theta_i^2 + \lambda|\theta_i| \end{split}$$

for all i = 1, ..., d. When $\widehat{\theta}_i^{OLS} \ge 0$, then $\widehat{\theta}_i \ge 0$ so

$$-2\widehat{\theta}_{i}^{OLS}\theta_{i}+\theta_{i}^{2}+\lambda|\theta_{i}|=-2\widehat{\theta}_{i}^{OLS}\theta_{i}+\theta_{i}^{2}+\lambda\theta_{i}$$

Differentiating with respect to θ_i , setting equal to zero, and solving gives

$$\widehat{\theta}_i = \left(\widehat{\theta}_i^{OLS} - \frac{\lambda}{2}\right) \mathbb{1}_{\widehat{\theta}_i^{OLS} \geq \frac{\lambda}{2}}.$$

When $\widehat{\theta}_i^{OLS} \leq 0$, the analogous steps give

$$\widehat{\theta}_i = \left(\widehat{\theta}_i^{OLS} + \frac{\lambda}{2}\right) \mathbb{1}_{\left\{\widehat{\theta}_i^{OLS} \le -\frac{\lambda}{2}\right\}},$$

Putting them together gives

$$\widehat{\theta}_{i} = \begin{cases} \widehat{\theta}_{i}^{OLS} - \frac{\lambda}{2} & \widehat{\theta}_{i}^{OLS} \geq \frac{\lambda}{2} \\ 0 & \widehat{\theta}_{i}^{OLS} \in \left(-\frac{\lambda}{2}, \frac{\lambda}{2}\right) \\ \widehat{\theta}_{i}^{OLS} + \frac{\lambda}{2} & \widehat{\theta}_{i}^{OLS} \leq \frac{\lambda}{2} \end{cases} .$$

(iii) Here the objective function is differentiable everywhere. Taking the gradient w.r.t. θ we have

$$\nabla_{\theta} \left(\sum_{i} (Y_i - \theta_i)^2 + \lambda \|\theta\|_2^2 \right) = \sum_{i} (-2Y_i \theta_i + 2\lambda \theta_i).$$

Setting this equal to 0 and solving for θ gives

$$\widehat{\theta_i} = \frac{Y_i}{1+\lambda}.\tag{3}$$

Since the objective is strictly convex, (3) is the unique solution.