# Introduction to Machine Learning
# Homework 1

March 19, 2019

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(1) Please follow the submission methods on the website;

(2) If you are not follow the methods or your submission format are not correct. we will deduct some score of your homework;

(3) Unless some special cases(such as illness), the submission over deadline will not be accepted and your score will be set as zero.

# 1 [20pts] Basic Probability and Statistics

The probability distribution of random variable $X$ follows:

$$f_X(x) = \begin{cases} \frac{1}{2} & 0 < x < 1; \\ \frac{1}{6} & 2 < x < 5; \\ 0 & \text{otherwise.} \end{cases} \tag{1.1}$$

(1) [5pts] Please give the cumulative distribution function $F_X(x)$ for X;

(2) [5pts] Define random variable $Y$ as $Y = 1/(X^2)$, please give the probability density function $f_Y(y)$ for $Y$;

(3) [10pts] For some random non-negative random variable Z, please prove the following two formulations are equivalent:

$$\mathbb{E}[Z] = \int_{z=0}^{\infty} z f(z) \mathrm{d}z, \tag{1.2}$$

$$\mathbb{E}[Z] = \int_{z=0}^{\infty} \Pr[Z \geq z] \mathrm{d}z, \tag{1.3}$$

Meantime, please calculate the expectation of random variable $X$ and $Y$ by these two expectation formulations to verify your proof.

(1) 按照定义，$F_X(x)$ 是 $f_X(x)$ 在 $x$ 定义域上的积分，所以 $F_X(x)$ 的函数表示为：

$$F_X(x) = \begin{cases} 0 & x \leq 0; \\ \frac{1}{2}x & 0 < x < 1; \\ \frac{1}{2} & 1 \leq x \leq 2; \\ \frac{1}{6}x + \frac{1}{6} & 2 < x < 5; \\ 1 & x \geq 5. \end{cases} \tag{1.4}$$

(2) 设 $Y$ 的累计分布函数为 $F_Y(y)$，则：

$$\begin{aligned} F_Y(y) &= \Pr[Y \leq y] \\ &= \Pr[\frac{1}{X^2} \leq y] \\ &= \Pr[X \geq \frac{1}{\sqrt{y}}] \\ &= 1 - F_X(\frac{1}{\sqrt{y}}) \end{aligned} \tag{1.5}$$

故 $Y$ 的概率密度函数为:

$$
\begin{aligned}
f_Y(y) &= \frac{\mathrm{d}F_Y(y)}{\mathrm{d}y} \\
&= \frac{1}{2} f_X(\frac{1}{\sqrt{y}}) y^{-\frac{3}{2}}
\end{aligned}
\tag{1.6}
$$

因此可得

$$
f_Y(y) = \begin{cases} \frac{1}{12} y^{-\frac{3}{2}} & \frac{1}{25} < y < \frac{1}{4}; \\ \frac{1}{4} y^{-\frac{3}{2}} & y > 1; \\ 0 & \text{otherwise.} \end{cases}
\tag{1.7}
$$

(3) 证明:

$$
\begin{aligned}
\int_{z=0}^{\infty} \Pr[Z \geq z] \mathrm{d}z &= \int_{z=0}^{\infty} \int_{x=z}^{\infty} f(x) \mathrm{d}x \mathrm{d}z \\
&= \int_{x=0}^{\infty} \int_{z=0}^{x} f(x) \mathrm{d}z \mathrm{d}x \\
&= \int_{z=0}^{\infty} z f(z) \mathrm{d}z
\end{aligned}
\tag{1.8}
$$

对于随机变量 $X$ ：

$$
\begin{aligned}
\int_{x=0}^{\infty} x f(x) \mathrm{d}x &= \int_{x=0}^{1} \frac{1}{2} x \mathrm{d}x + \int_{x=2}^{5} \frac{1}{6} x \mathrm{d}x = 2 \\
\int_{x=0}^{\infty} \Pr[X \geq x] \mathrm{d}x &= \int_{x=0}^{\infty} 1 - F_X(x) \mathrm{d}x \\
&= \int_{x=0}^{1} 1 - \frac{1}{2} x \mathrm{d}x + \int_{x=1}^{2} \frac{1}{2} \mathrm{d}x + \int_{x=2}^{5} \frac{5}{6} - \frac{1}{6} x \mathrm{d}x \\
&= 2
\end{aligned}
\tag{1.9}
$$

对于随机变量 $Y$ ：

$$
\begin{aligned}
\int_{y=0}^{\infty} y f(y) \mathrm{d}y &= \int_{y=\frac{1}{25}}^{\frac{1}{4}} \frac{1}{12} y^{-\frac{1}{2}} \mathrm{d}y + \int_{y=1}^{\infty} \frac{1}{4} y^{-\frac{1}{2}} \mathrm{d}y = \infty \\
\int_{y=0}^{\infty} \Pr[Y \geq y] \mathrm{d}y &= \int_{y=0}^{\infty} 1 - F_Y(y) \mathrm{d}y \\
&= \int_{y=0}^{\infty} F_X(\frac{1}{\sqrt{y}}) \mathrm{d}y \\
&= \int_{y=0}^{\frac{1}{25}} 1 \mathrm{d}y + \int_{y=\frac{1}{25}}^{\frac{1}{4}} \frac{1}{6\sqrt{y}} + \frac{1}{6} \mathrm{d}y + \int_{y=\frac{1}{4}}^{1} \frac{1}{2} \mathrm{d}y + \int_{y=1}^{\infty} \frac{1}{2\sqrt{y}} \mathrm{d}y \\
&= \infty
\end{aligned}
\tag{1.10}
$$

故得证。

## 2 [20pts] Strong Convexity

Let $D \in \mathbb{R}^2$ be a finite set. Define a function $E : \mathbb{R}^3 \to \mathbb{R}$ by

$$E(a,b,c) = \sum_{x \in \mathcal{D}} (ax_1^2 + bx_1 + c - x_2)^2. \tag{2.1}$$

(1) [10pts] Show that $E$ is convex.

(2) [10pts] Does there exist a set $D$ such that $E$ is strongly convex? Proof or a counterexample.

(1) 函数 $E(a,b,c) = \sum_{x \in \mathcal{D}} (ax_1^2 + bx_1 + c - x_2)^2$ 的 Hessian 矩阵为：

$$H = \begin{bmatrix} 2\sum_{x\in\mathcal{D}} x_1^4 & 2\sum_{x\in\mathcal{D}} x_1^3 & 2\sum_{x\in\mathcal{D}} x_1^2 \\ 2\sum_{x\in\mathcal{D}} x_1^3 & 2\sum_{x\in\mathcal{D}} x_1^2 & 2\sum_{x\in\mathcal{D}} x_1 \\ 2\sum_{x\in\mathcal{D}} x_1^2 & 2\sum_{x\in\mathcal{D}} x_1 & 2\sum_{x\in\mathcal{D}} 1 \end{bmatrix} \tag{2.2}$$

即证矩阵 $H$ 是半正定的，这等价于证明矩阵 $H$ 的各阶顺序主子式均非负。而矩阵 $H$ 的各阶顺序主子式依次为：

$$\left| 2\sum_{x\in\mathcal{D}} x_1^4 \right| \geq 0 \tag{2.3}$$

由柯西-施瓦茨不等式，可知对欧几里得空间 $\mathrm{R}^n$：

$$(x_1^2 + x_2^2 + \cdots + x_n^2)(y_1^2 + y_2^2 + \cdots + y_n^2) \geq (x_1y_1 + x_2y_2 + \cdots + x_ny_n)^2 \tag{2.4}$$

当 $\frac{x_1}{y_1} = \frac{x_2}{y_2} = \cdots = \frac{x_n}{y_n}$ 时等式成立。

因此

$$\begin{vmatrix} 2\sum_{x\in\mathcal{D}} x_1^4 & 2\sum_{x\in\mathcal{D}} x_1^3 \\ 2\sum_{x\in\mathcal{D}} x_1^3 & 2\sum_{x\in\mathcal{D}} x_1^2 \end{vmatrix} = 4\left(\sum_{x\in\mathcal{D}} x_1^4 * \sum_{x\in\mathcal{D}} x_1^2 - \left(\sum_{x\in\mathcal{D}} x_1^3\right)^2\right) \geq 0 \tag{2.5}$$

$$\begin{aligned} \begin{vmatrix} 2\sum_{x\in\mathcal{D}} x_1^4 & 2\sum_{x\in\mathcal{D}} x_1^3 & 2\sum_{x\in\mathcal{D}} x_1^2 \\ 2\sum_{x\in\mathcal{D}} x_1^3 & 2\sum_{x\in\mathcal{D}} x_1^2 & 2\sum_{x\in\mathcal{D}} x_1 \\ 2\sum_{x\in\mathcal{D}} x_1^2 & 2\sum_{x\in\mathcal{D}} x_1 & 2\sum_{x\in\mathcal{D}} 1 \end{vmatrix} &= 4\Big(\sum_{x\in\mathcal{D}} x_1^4 * \sum_{x\in\mathcal{D}} x_1^2 * \sum_{x\in\mathcal{D}} 1 + \sum_{x\in\mathcal{D}} x_1^3 * \sum_{x\in\mathcal{D}} x_1 * \sum_{x\in\mathcal{D}} x_1^2 \\ &\quad + \sum_{x\in\mathcal{D}} x_1^2 * \sum_{x\in\mathcal{D}} x_1^3 * \sum_{x\in\mathcal{D}} x_1 - \sum_{x\in\mathcal{D}} x_1^4 * \sum_{x\in\mathcal{D}} x_1 * \sum_{x\in\mathcal{D}} x_1 \\ &\quad - \sum_{x\in\mathcal{D}} x_1^3 * \sum_{x\in\mathcal{D}} x_1^3 * \sum_{x\in\mathcal{D}} 1 - \sum_{x\in\mathcal{D}} x_1^2 * \sum_{x\in\mathcal{D}} x_1^2 * \sum_{x\in\mathcal{D}} x_1^2\Big) \\ &\geq 0 \end{aligned} \tag{2.6}$$

因此可得矩阵 $H$ 是半正定的，故 $E$ 是凸函数。

(2) 存在集合 $D$ 使得 $E$ 是严格凸函数。从 (1) 中可知矩阵 $H$ 的二三阶顺序主子式等号成立的条件是对于所有 $x \in \mathcal{D}$，$x_1$ 均相等。显然只需要构造 $\mathcal{D} = \{(1,2),(3,4)\}$，即可得 $H$ 的二三阶顺序主子式均大于 0 ，此时 $H$ 是正定矩阵，即 $E$ 是凸函数。

# 3 [20pts] Transition Probability Matrix

Suppose $x_k$ is the fraction of NJU students who prefer course A at year $k$. The remaining fraction $y_k = 1 - x_k$ prefers course B.

At year $k+1$, $\frac{1}{5}$ of those who prefer course A change their mind. Also at the same year, $\frac{1}{10}$ of those who prefer course B change their mind (possibly after taking the problem 3 last year).

Create the matrix P to give $[x_{k+1} \quad y_{k+1}]^\top = P[x_k \quad y_k]^\top$ and find the limit of $P^k[1 \quad 0]^\top$ as $k \to \infty$.

由题意可知

$$x_{k+1} = \frac{4}{5}x_k + \frac{1}{10}y_k \tag{3.1}$$

$$y_{k+1} = \frac{9}{10}y_k + \frac{1}{5}x_k \tag{3.2}$$

因此

$$P = \begin{bmatrix} \frac{4}{5} & \frac{1}{10} \\ \frac{1}{5} & \frac{9}{10} \end{bmatrix} \tag{3.3}$$

矩阵 $P$ 的特征多项式为

$$P - \lambda I = \begin{vmatrix} \frac{4}{5} - \lambda & \frac{1}{10} \\ \frac{1}{5} & \frac{9}{10} - \lambda \end{vmatrix} \tag{3.4}$$

令多项式为 0 ，解得特征值 $\lambda = 1$ 和 $\lambda = 0.7$
特征值 $\lambda = 1$ 对应的特征向量为 $[2 \quad 1]^\top$, $\lambda = 0.7$ 对应的特征向量为 $[1 \quad -1]^\top$，故可知矩阵对角化时所用的 $Q$ 与 $Q^{-1}$ 分别为：

$$Q = \begin{bmatrix} 2 & 1 \\ 1 & -1 \end{bmatrix} \tag{3.5}$$

$$Q^{-1} = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & -\frac{2}{3} \end{bmatrix} \tag{3.6}$$

于是可知矩阵 $P$ 的对角化结果为

$$\begin{bmatrix} 1 & 0 \\ 0 & 0.7 \end{bmatrix} = D = Q^{-1}PQ \tag{3.7}$$

所以有

$$P = QDQ^{-1} \Rightarrow P^k = QD^kQ^{-1} \tag{3.8}$$

$$\lim_{k\to\infty} P^k = \lim_{k\to\infty} QD^kQ^{-1} = Q\left(\lim_{k\to\infty} D^k\right)Q^{-1} \tag{3.9}$$

故

$$\lim_{k\to\infty} P^k = \begin{bmatrix} \frac{2}{3} & \frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} \end{bmatrix} \tag{3.10}$$

因此

$$\lim_{k\to\infty} P^k[1 \quad 0]^\top = [\frac{2}{3} \quad \frac{1}{3}]^\top \tag{3.11}$$

# 4 [20pts] Hypothesis Testing

Yesterday, a student was caught by the teacher when tossing a coin in class. The teacher is very nice and did not want to make things difficult. S(he) wished the student to determine *if the coin is biased for heads* with $\alpha = 0.05$.

Also, according to the student's desk mate, the coin was tossed for 50 times and it got 35 heads.

(1) [10pts] Show all calculate and rules (hint: using z-test).

(2) [10pts] Calculate the p-value and interpret it.

(1) 记原假设 $H0$ 为"硬币正面不偏重"，备择假设 $H1$ 为"硬币正面偏重"。抛硬币本身属于二项分布，即 $X \sim B(n, 0.5)$ ，由题意可知 $n = 50$，属于大样本，故可用正态分布来近似，得到：

$$z = \frac{p - 0.5}{\sqrt{\frac{0.5*(1-0.5)}{n}}} = \frac{p - 0.5}{0.5}\sqrt{n} \sim N(0,1) \tag{4.1}$$

将 $p = \frac{35}{50} = 0.7$ 代入，可得 $z = 2\sqrt{2} \approx 2.83$，查表可知 $z_{1-\alpha} = z_{0.95} \approx 1.65 < 2.83$，落入拒绝域，因此原假设不成立，即硬币正面偏重。

(2)

$$p = P(Z > z) = P(Z > 2.83) = 1 - \Phi(2.83) = 0.0023 \tag{4.2}$$

$p$ 值的意思是当原假设为真的条件下，检验统计量的观察值大于或等于其计算值的概率。此处 $p$ 值指的是在硬币正面不偏重的情况下，$z$ 值大于 2.83 的概率。因为 $p = 0.0023 < 0.05 = \alpha$，所以拒绝原假设。

## 5 [20pts] Performance Measures

We have a set of samples that we wish to classify in one of two classes and a ground truth class of each sample (denoted as 0 and 1). For each example a classifier gives us a score (score closer to 0 means class 0, score closer to 1 means class 1). Below are the results of two classifiers ($C_1$ and $C_2$) for 8 samples,their ground truth values ($y$) and the score values for both classifiers ($y_{C_1}$ and $y_{C_2}$).

| $y$ | 1 | 0 | 1 | 1 | 1 | 0 | 0 | 0 |
|---|---|---|---|---|---|---|---|---|
| $y_{C_1}$ | 0.5 | 0.3 | 0.6 | 0.22 | 0.4 | 0.51 | 0.2 | 0.33 |
| $y_{C_2}$ | 0.04 | 0.1 | 0.68 | 0.22 | 0.4 | 0.11 | 0.8 | 0.53 |

(1) [8pts] For the example above calculate and draw the ROC curves for classifier $C_1$ and $C_2$. Also calculate the area under the curve (AUC) for both classifiers.

(2) [8pts] For the classifier $C_1$ select a decision threshold $th_1 = 0.33$ which means that $C_1$ classifies a sample as class 1, if its score $y_{C_1} > th_1$, otherwise it classifies it as class 0. Use it to calculate the confusion matrix and the $F_1$ score. Do the same thing for the classifier $C_2$ using a threshold value $th_2 = 0.1$.

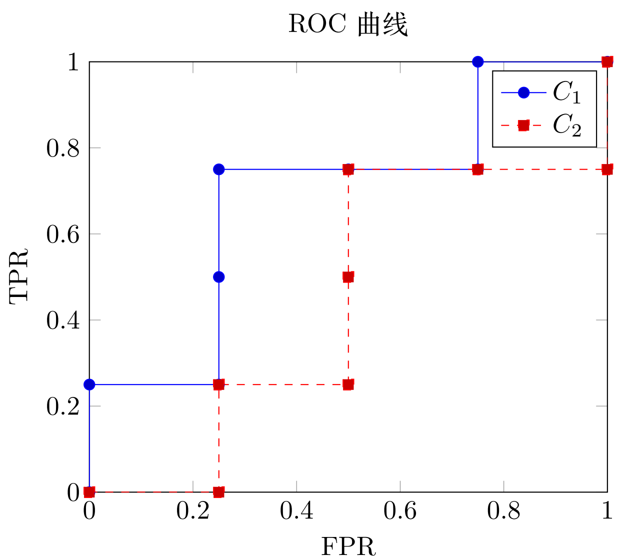
(3) [4pts] Prove Eq.(2.22) in Page 35. (AUC $= 1 - \ell_{rank}$).

(1) 将 $y_{C_1}$ 与 $y_{C_2}$ 的数据按分数从大到小排序可得表 1

| $C_1$ | | $C_2$ | |
|---|---|---|---|
| y | $y_{C_1}$ | y | $y_{C_2}$ |
| 1 | 0.6 | 0 | 0.8 |
| 0 | 0.51 | 1 | 0.68 |
| 1 | 0.5 | 0 | 0.53 |
| 1 | 0.4 | 1 | 0.4 |
| 0 | 0.33 | 1 | 0.22 |
| 0 | 0.3 | 0 | 0.11 |
| 1 | 0.22 | 0 | 0.1 |
| 0 | 0.2 | 1 | 0.04 |

Table 1: $C_1$ 与 $C_2$ 的分数结果排序

根据表 1 分别计算分类器 $C_1$ 与 $C_2$ 的 TPR 与 FPR，可得各自的 ROC 曲线为:




$$
\begin{aligned}
AUC_{C_1} &= 0.25 * 0.25 + 0.75 * (0.75 - 0.25) + 1 * (1 - 0.75) = 0.6875 \\
AUC_{C_2} &= 0.25 * (0.5 - 0.25) + 0.75 * (1 - 0.5) = 0.4375
\end{aligned} \tag{5.1}
$$

(2) 分别计算分类器 $C_1$ 与 $C_2$ 的混淆矩阵，可得：

$C_1$ 的混淆矩阵：

| | | Actual Class | |
|---|---|---|---|
| | | 1 | 0 |
| Predicted | 1 | 3 | 2 |
| Class | 0 | 1 | 2 |

$C_2$ 的混淆矩阵：

| | | Actual Class | |
|---|---|---|---|
| | | 1 | 0 |
| Predicted | 1 | 3 | 4 |
| Class | 0 | 1 | 0 |

分别计算分类器 $C_1$ 与 $C_2$ 的 F 分数，可得：

$$
\begin{aligned}
F_{1_{C_1}} &= 2 * \frac{0.6 * 0.75}{0.6 + 0.75} = 0.67 \\
F_{1_{C_2}} &= 2 * \frac{0.43 * 0.75}{0.43 + 0.75} = 0.55
\end{aligned} \tag{5.2}
$$

(3) 由 AUC 定义可知 $1-\mathrm{AUC}$ 即 ROC 曲线以上的面积。设 $S^+$ 为正例的序号集合，$S^-$ 为负例的序号集合，则

$$
\begin{aligned}
1-\mathrm{AUC} &= \frac{1}{2}\sum_{i=1}^{m-1}\left(x_i + x_{i+1}\right)\left(y_{i+1} - y_i\right) \\
&= \frac{1}{m^+}\sum_{i\in S^+} x_i + 0\sum_{i\in S^-} x_i \\
&= \frac{1}{m^+}\sum_{i\in S^+} x_i \\
&= \frac{1}{m^+}\sum_{i\in S^+}\frac{1}{m^-}\sum_{j\in S^-}\left(\mathbb{I}(f(x_i) < f(x_j)) + \frac{1}{2}\mathbb{I}(f(x_i) = f(x_j))\right) \\
&= \frac{1}{m^+m^-}\sum_{x^+\in D^+}\sum_{x^-\in D^-}\left(\mathbb{I}(f(x^+) < f(x^-)) + \frac{1}{2}\mathbb{I}(f(x^+) = f(x^-))\right) \\
&= l_{rank}
\end{aligned} \tag{5.3}
$$

第 1 个等号代表从水平方向逐步增加 ROC 曲线以上的面积，第 2 个等号表明负例集合增加的单位直线没有增加 ROC 曲线以上的面积。
因此 $\mathrm{AUC} = 1 - \ell_{rank}$ 成立。

# 6 [Bonus 10pts]Expected Prediction Error

For least squares linear regression problem, we assume our linear model as:

$$
y = x^T\beta + \epsilon, \tag{6.1}
$$

where $\epsilon$ is noise and follows $\epsilon \sim N(0, \sigma^2)$. Note the instance feature of training data $\mathcal{D}$ as $\boldsymbol{X} \in \mathbb{R}^{p\times n}$ and note the label as $\boldsymbol{Y} \in \mathbb{R}^n$, where $n$ is the number of instance and $p$ is the feature dimension. So the estimation of model parameter is:

$$
\hat{\beta} = (\boldsymbol{X}\boldsymbol{X}^T)^{-1}\boldsymbol{X}\boldsymbol{Y}. \tag{6.2}
$$

For some given test instance $x_0$, please proof the expected prediction error $\mathbf{EPE}(x_0)$ follows:

$$
\mathbf{EPE}(x_0) = \sigma^2 + \mathbb{E}_{\mathcal{D}}[x_0^T(\boldsymbol{X}\boldsymbol{X}^T)^{-1}x_0\sigma^2]. \tag{6.3}
$$

Please give the steps and details of your proof.(Hint: $\mathbf{EPE}(x_0) = \mathbb{E}_{y_0|x_0}\mathbb{E}_{\mathcal{D}}[(y_0 - \hat{y}_0)^2]$, you can also refer to the proof progress of variance-bias decomposition on the page 45 of our reference book)

根据 $E(f;D) = bias^2(x) + var(x) + \epsilon^2$ 即
$E(f;D) = \mathbb{E}_D[(f(x;D) - \bar{f}(x))^2] + (\bar{f}(x) - y)^2 + \mathbb{E}_D[(y_D - y)^2]$
可知

$$\begin{aligned}\mathbf{EPE}(x_0) &= \mathbb{E}_{y_0|x_0}\mathbb{E}_{\mathcal{D}}[(y_0 - \hat{y}_0)^2] \\ &= \mathbb{E}_{y_0|x_0}\mathbb{E}_{\mathcal{D}}[(y_0 - y)^2] + \mathbb{E}_{y_0|x_0}[(\bar{\hat{y}}_0 - y)^2] + \mathbb{E}_{y_0|x_0}\mathbb{E}_{\mathcal{D}}[(\hat{y}_0 - \bar{\hat{y}}_0)^2] \\ &= \sigma^2 + 0 + \mathbb{E}_{\mathcal{D}}[(\hat{y}_0 - \bar{\hat{y}}_0)^2]\end{aligned} \tag{6.4}$$

即证

$$\mathbb{E}_{\mathcal{D}}[(\hat{y}_0 - \bar{\hat{y}}_0)^2] = \mathbb{E}_{\mathcal{D}}[x_0^T(\boldsymbol{X}\boldsymbol{X}^T)^{-1}x_0\sigma^2] \tag{6.5}$$