CSC 665: Calibration Homework

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Please complete the following set of exercises **on your own**. The homework is due **on Sep 3, in class**. You may find the following version of Taylor's Theorem in multivariate calculus helpful:

Theorem 1. *Suppose f is twice differentiable in $\mathbb{R}^d$. Then given two points a, b in $\mathbb{R}^d$, there exists some t in $[0,1]$, such that*

$$f(b) = f(a) + \langle \nabla f(a), b - a \rangle + \frac{1}{2}(b-a)^\top \nabla^2 f(\xi)(b-a),$$

where $\xi = ta + (1-t)b$. Here $\nabla f(x) \triangleq (\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_d})$ is the gradient of f at x, and

$$\nabla^2 f(x) \triangleq \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ & \cdots & \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix}$$

is the Hessian of f at x.

Problem 1

Denote by $\mathrm{B}(n,p)$ the binomial distribution with n being the number of trials, and p being the success probability of each trial, and denote by $\mathrm{N}(\mu, \sigma^2)$ the normal distribution with mean μ and variance σ^2.

1. Suppose Y is a random variable such that $P(Y = +1) = P(Y = -1) = \frac{1}{2}$. In addition, given Y, X has the following conditional probability distribution: given $Y = -1$, $X \sim \mathrm{B}(3, \frac{2}{3})$; given $Y = +1$, $X \sim \mathrm{B}(2, \frac{1}{3})$. Calculate:
   (a) the joint probability table of (X, Y);
   (b) $P(Y = 1|X = 3)$;
   (c) $P(Y = -1|X = 1)$.

2. Suppose Y is a random variable such that $P(Y = +1) = P(Y = -1) = \frac{1}{2}$. In addition, suppose given Y, X has the following conditional probability distribution: given $Y = -1$, $X \sim \mathrm{N}(\mu_-, \sigma^2)$; given $Y = +1$, $X \sim \mathrm{N}(\mu_+, \sigma^2)$. Define

   $$P(Y = +1|x) \triangleq \frac{P(Y = +1)p_{+1}(x)}{P(Y = +1)p_{+1}(x) + P(Y = -1)p_{-1}(x)}.$$

   where p_{+1} and p_{-1} are the conditional probability density functions of X given $Y = +1$ and $Y = -1$ respectively. Show that

   $$P(Y = +1|x) = \frac{1}{1 + \exp\Big(-\frac{\mu_+ - \mu_-}{\sigma^2} \cdot (x - \frac{\mu_+ + \mu_-}{2})\Big)}.$$

   (Remark: $P(Y = +1|x)$ has the intuitive interpretation that it is the conditional probability of $Y = +1$ given $X = x$. It can be shown rigorously that $P(Y = +1|x) = \lim_{\epsilon \to 0} P(Y = +1|X \in [x - \epsilon, x + \epsilon])$.)

Solution

1. (a) The joint probability table is

	$X=0$	$X=1$	$X=2$	$X=3$
$Y=-1$	$\frac{1}{54}$	$\frac{1}{9}$	$\frac{2}{9}$	$\frac{4}{27}$
$Y=+1$	$\frac{2}{9}$	$\frac{2}{9}$	$\frac{1}{18}$	0

(b)

$$P(Y=1|X=3) = \frac{P(Y=1,X=3)}{P(X=3)} = \frac{P(Y=1,X=3)}{P(Y=1,X=3)+P(Y=-1,X=3)} = \frac{0}{0+\frac{4}{27}} = 0.$$

(c)

$$P(Y=-1|X=1) = \frac{P(Y=-1,X=1)}{P(X=1)} = \frac{P(Y=-1,X=1)}{P(Y=1,X=1)+P(Y=-1,X=1)} = \frac{\frac{1}{9}}{\frac{1}{9}+\frac{2}{9}} = \frac{2}{3}.$$

2. Recall that by the definition of normal distribution, $p_{+1}(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\Big\{-\frac{(x-\mu_+)^2}{2\sigma^2}\Big\}$, and $p_{-1}(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\Big\{-\frac{(x-\mu_-)^2}{2\sigma^2}\Big\}$.

   Therefore, $p_{+1}(x)/p_{-1}(x) = \exp\Big\{-\frac{(x-\mu_+)^2-(x-\mu_-)^2}{2\sigma^2}\Big\} = \exp\Big\{-\frac{(\mu_+-\mu_-)(x-\frac{\mu_++\mu_-}{2})}{\sigma^2}\Big\}$.

   In addition, $P(Y=+1)=P(Y=-1)=\frac{1}{2}$. Therefore,

$$\begin{aligned} P(Y=+1|x) &= \frac{P(Y=+1)p_{+1}(x)}{P(Y=+1)p_{+1}(x)+P(Y=-1)p_{-1}(x)} \\ &= \frac{p_{+1}(x)}{p_{+1}(x)+p_{-1}(x)} \\ &= \frac{1}{1+\frac{p_{+1}(x)}{p_{-1}(x)}} \\ &= \frac{1}{1+\exp\Big\{-\frac{(\mu_+-\mu_-)(x-\frac{\mu_++\mu_-}{2})}{\sigma^2}\Big\}}. \end{aligned}$$

Problem 2

1. Suppose $D = \mathrm{U}([0,1])$, i.e. the uniform distribution over the $[0,1]$ interval. Consider a set of samples $S = (X_1, \ldots, X_n)$ drawn identically and independently from distribution D.

   Write a program that plots the empirical *cumulative distribution function* (CDF) of the sample S, that is,

$$F_n(t) = \frac{1}{n}\sum_{i=1}^{n}\mathbf{1}(x_i \le t), t \in \mathbb{R},$$

   where

$$\mathbf{1}(A) = \begin{cases} 1 & A \text{ is true} \\ 0 & A \text{ is false} \end{cases}$$

is the indicator function. You may use any programming languages you like (e.g. Python and Jupyter notebook).

Draw two sets of samples S_1 and S_2 of size $n = 5$. Plot F_n^1, the CDF of S_1, and plot F_n^2, the CDF of S_2. Are they different? Why?

2. Repeat the same experiment in for $n = 100$ and $n = 1000$. Do the F_n^1 and F_n^2 functions become closer as n increases?

3. In the above experiment, as n goes to infinity, what function does F_n converge to? Can you derive a formula for that function (denoted as F)?

4. Suppose D is the the standard normal distribution $\mathrm{N}(0, 1)$, what function does F_n converge to?

Solution

1. See Figure 1 below. (The exact results depend on the random points drawn - they can vary case by case.) They are different. As S_1 and S_2 are two different samples, their induced CDFs would also be different.

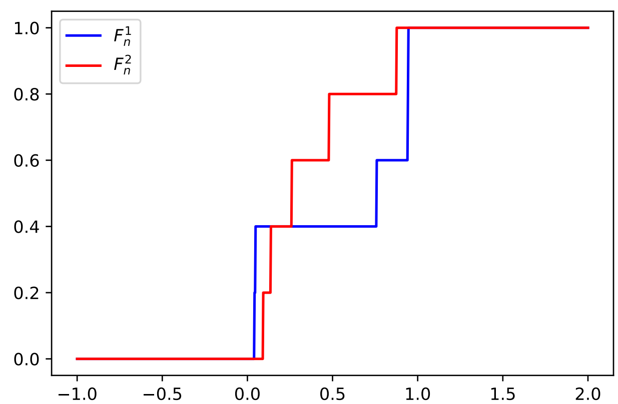

Figure 1: A random draw of F_n^1 and F_n^2 with sample size $n = 5$.

2. See Figures 2 and 3 below. Yes, F_n^1 and F_n^2 do become closer as n increases. (Of course, in some extremely unlikely draws of random samples, they *can* become farther away as n increases.)

3. By the (weak) law of large numbers, for every t in $\mathbb{R}$, $F_n(t) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}(x_i \leq t) \to F(t) = \mathbb{P}(X \leq t)$ (in probability).

$$F(t) = \mathbb{P}(X \leq t) = \begin{cases} 0 & t \leq 0 \\ t & 0 < t < 1 \\ 1 & t \geq 1 \end{cases}.$$

4. When X is drawn from the standard normal distribution,

$$F(t) = \mathbb{P}(X \leq t) = \int_{-\infty}^{t} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx.$$

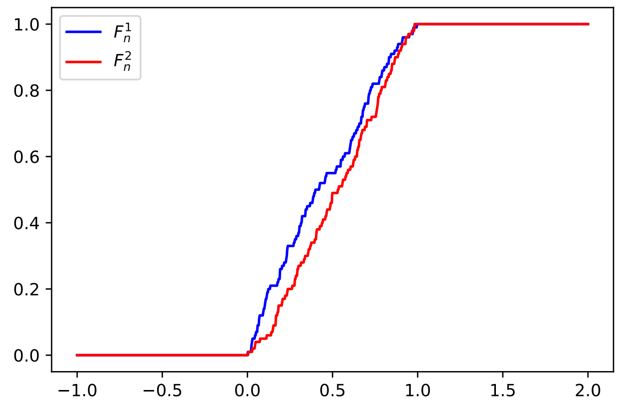

Figure 2: A random draw of F_n^1 and F_n^2 with sample size $n = 100$.

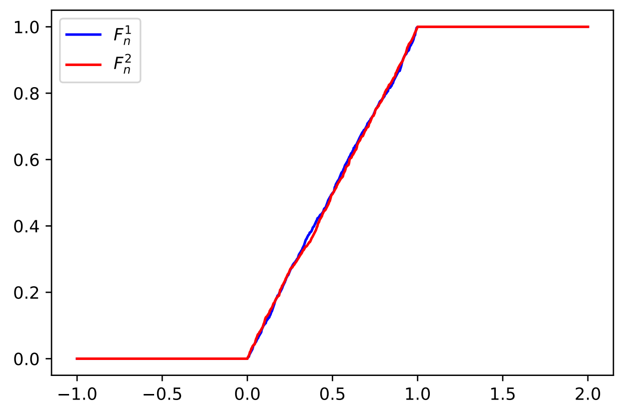

Figure 3: A random draw of F_n^1 and F_n^2 with sample size $n = 1000$.

Problem 3

1. Define function
$$h(x) \triangleq x \ln x + (1-x)\ln(1-x), x \in (0,1).$$
Show that for any p and q in $(0,1)$,
$$h(p) - h(q) - h'(q)(p-q) = p \ln \frac{p}{q} + (1-p)\ln\frac{1-p}{1-q}.$$
(Remark: the expression on the right hand side is often called the *binary relative entropy*, denoted as $\mathrm{kl}(p,q)$; the h function is often called the *negative binary entropy*.)

2. Suppose $0 < p < q < 1$. Use Taylor's Theorem to show that
$$\mathrm{kl}(p,q) \geq 2(p-q)^2.$$
Furthermore, show that
$$\mathrm{kl}(p,q) \geq \frac{(p-q)^2}{2q}.$$

3. Define the m-dimensional probability simplex Δ^{m-1} as $\left\{p \in \mathbb{R}^m : \text{ for all } i, p_i \geq 0, \sum_{i=1}^m p_i = 1\right\}$. For two vectors p, q in Δ^{m-1}, define the negative entropy of p as:

$$\mathrm{H}(p) \triangleq \sum_{i=1}^m p_i \ln p_i,$$

and the relative entropy between p and q as:

$$\mathrm{KL}(p, q) \triangleq \sum_{i=1}^m p_i \ln \frac{p_i}{q_i}.$$

Verify that

$$\mathrm{H}(p) - \mathrm{H}(q) - \left\langle \nabla \mathrm{H}(q), p - q \right\rangle = \mathrm{KL}(p, q).$$

4. Using Taylor's Theorem, show that for any p, q in Δ^{m-1}, $\mathrm{KL}(p, q) \geq 0$. Furthermore, show that $\mathrm{KL}(p, q) \geq \frac{1}{2}(\sum_{i=1}^m |p_i - q_i|)^2$.

Hint: at some point, you may want to use the following variant of Cauchy-Schwarz inequality:

$$(\sum_{i=1}^m y_i) \cdot (\sum_{i=1}^m \frac{x_i^2}{y_i}) \geq (\sum_{i=1}^m |x_i|)^2.$$

Solution

1. Observe that $h'(x) = (1 + \ln x) - (1 + \ln(1 - x)) = \ln x - \ln(1 - x)$.

Therefore, for any p and q in $(0, 1)$,

$$\begin{aligned} h(p) - h(q) - h'(q)(p - q) &= h(p) - (h(q) + h'(q)(p - q)) \\ &= p \ln p + (1 - p) \ln(1 - p) - (q \ln q + (1 - q) \ln(1 - q) + (p - q)(\ln q - \ln(1 - q)) \\ &= p \ln p + (1 - p) \ln(1 - p) - (p \ln q + (1 - p) \ln(1 - q)) \\ &= p \ln \frac{p}{q} + (1 - p) \ln \frac{1 - p}{1 - q}. \end{aligned}$$

2. Observe that $h(x)$ is twice differentiable on $(0, 1)$. Then, by Talyor's Theorem, for any p, q,

$$\mathrm{kl}(p, q) = h(p) - h(q) - h'(q)(p - q) = \frac{1}{2} h''(\xi)(p - q)^2,$$

for some $\xi = (1 - t)p + tq$, where $t \in [0, 1]$. As both p and q are in $(0, 1)$, $\xi \in (p, q) \subset (0, 1)$.

Now, observe that for all x in $(0, 1)$, $h''(x) = \frac{1}{x} + \frac{1}{1-x} = \frac{1}{x(1-x)} \geq \frac{1}{((1-x+x)/2)^2} = 4$, This implies that

$$\mathrm{kl}(p, q) = \frac{1}{2} h''(\xi)(p - q)^2 \geq \frac{1}{2} \cdot 4(p - q)^2 = 2(p - q)^2.$$

The second inequality follows from the fact that $h''(\xi) = \frac{1}{\xi(1-\xi)} \geq \frac{1}{\xi} \geq \frac{1}{q}$. This implies that

$$\mathrm{kl}(p, q) = \frac{1}{2} h''(\xi)(p - q)^2 \geq \frac{(p - q)^2}{2q}.$$

3. Observe that $\nabla \mathrm{H}(q) = (\frac{\partial H}{\partial x_1}, \ldots, \frac{\partial H}{\partial x_m}) = (1 + \ln q_1, \ldots, 1 + \ln q_m)$.

$$\begin{aligned}
\mathrm{H}(p)-\mathrm{H}(q)-\left\langle\nabla \mathrm{H}(q), p-q\right\rangle &= \sum_{i=1}^{m} p_i \ln p_i - \sum_{i=1}^{m} q_i \ln q_i - \sum_{i=1}^{m}(p_i - q_i)(1+\ln q_i) \\
&= \sum_{i=1}^{m}(p_i \ln p_i - q_i \ln q_i - (p_i - q_i)\ln q_i) - \sum_{i=1}^{m}(p_i - q_i) \\
&= \sum_{i=1}^{m} p_i \ln \frac{p_i}{q_i} - \sum_{i=1}^{m}(p_i - q_i),
\end{aligned}$$

As both p_i and q_i are in Δ^{m-1}, $\sum_{i=1}^m p_i = \sum_{i=1}^m q_i = 1$. Therefore,

$$\mathrm{H}(p)-\mathrm{H}(q)-\left\langle\nabla \mathrm{H}(q), p-q\right\rangle = \sum_{i=1}^{m} p_i \ln \frac{p_i}{q_i} = \mathrm{KL}(p,q).$$

4. Observe that $H(p)$ is twice differentiable on $(0,1)^m$. Then, by Talyor's Theorem, for any p, q in $(0,1)^m$,

$$\mathrm{H}(p)-\mathrm{H}(q)-\left\langle\nabla \mathrm{H}(q), p-q\right\rangle = \frac{1}{2}(p-q)^\top \nabla^2 \mathrm{H}(\xi)(p-q).$$

for some $\xi = (1-t)p + tq$ and $t \in [0,1]$.

Here, the entries of Hessian of H can be written as the following:

$$(\nabla^2 \mathrm{H}(x))_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j} = \begin{cases} \frac{1}{x_i}, & i=j \\ 0, & i \neq j \end{cases}.$$

Now, for p and q in Δ^{m-1}, we have that

$$\begin{aligned}
\mathrm{KL}(p,q) &= \mathrm{H}(p)-\mathrm{H}(q)-\left\langle\nabla \mathrm{H}(q), p-q\right\rangle \\
&= \frac{1}{2}(p-q)^\top \nabla^2 \mathrm{H}(\xi)(p-q) \\
&= \frac{1}{2}\sum_{i=1}^{m} \frac{(p_i-q_i)^2}{\xi_i}, \qquad (1)
\end{aligned}$$

for some $\xi = (1-t)p + tq$ and $t \in [0,1]$. Specifically, all ξ_i's are nonnegative, and $\sum_{i=1}^m \xi_i = (1-t)\sum_{i=1}^m p_i + t\sum_{i=1}^m q_i = 1$. As all the terms in the sum are nonnegative, $\mathrm{KL}(p,q) \geq 0$.

Now, applying the (variant of) Cauchy-Schwarz Inequality, we get

$$\begin{aligned}
\sum_{i=1}^{m} \frac{(p_i-q_i)^2}{\xi_i} &= (\sum_{i=1}^{m} \xi_i) \cdot (\sum_{i=1}^{m} \frac{(p_i-q_i)^2}{\xi_i}) \\
&\geq (\sum_{i=1}^{m} |p_i - q_i|)^2.
\end{aligned}$$

Plugging this inequality into Equation (1), we conclude that $\mathrm{KL}(p,q) \geq \frac{1}{2}(\sum_{i=1}^m |p_i - q_i|)^2$.