Chapter 1 Introduction

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1.2 Probability Theory

(1.39)

$$\begin{aligned} \text{var}[f] &= \mathbb{E}[(f(x) - \mathbb{E}[f(x)])^2] \\ &= \mathbb{E}[f(x)^2 - 2\mathbb{E}[f(x)]f(x) + \mathbb{E}[f(x)]^2] \\ &= \mathbb{E}[f(x)^2] - \mathbb{E}[2\mathbb{E}[f(x)]f(x)] + \mathbb{E}[\mathbb{E}[f(x)]^2] \\ &= \mathbb{E}[f(x)^2] - 2\mathbb{E}[f(x)]^2 + \mathbb{E}[f(x)]^2 \\ &= \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2. \end{aligned}$$

(1.48)

Denote

$$I = \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}x^2\right) dx,\tag{*}$$

then

$$I^{2} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^{2}}x^{2} - \frac{1}{2\sigma^{2}}y^{2}\right) dx dy.$$

Applying the transformation $x = r \cos \theta$, $y = r \sin \theta$, and making use of (1.27), we have

$$I^{2} = \int_{0}^{2\pi} \int_{0}^{\infty} \exp\left(-\frac{1}{2\sigma^{2}} (r\cos\theta)^{2} - \frac{1}{2\sigma^{2}} (r\sin\theta)^{2}\right) \left|\frac{\partial(x,y)}{\partial(r,\theta)}\right| dr d\theta$$
$$= \int_{0}^{2\pi} \int_{0}^{\infty} \exp\left(-\frac{r^{2}}{2\sigma^{2}}\right) r dr d\theta.$$

Then, by substituting $u = r^2$, we obtain

$$I^{2} = \int_{0}^{2\pi} \int_{0}^{\infty} \exp\left(-\frac{u}{2\sigma^{2}}\right) u^{1/2} \left| \frac{\mathrm{d}r}{\mathrm{d}u} \right| \mathrm{d}u \,\mathrm{d}\theta$$
$$= \int_{0}^{2\pi} \int_{0}^{\infty} \frac{1}{2} \exp\left(-\frac{u}{2\sigma^{2}}\right) \mathrm{d}u \,\mathrm{d}\theta$$
$$= -\sigma^{2} \exp\left(-\frac{u}{2\sigma^{2}}\right) \Big|_{0}^{\infty} \int_{0}^{2\pi} \mathrm{d}\theta$$
$$= 2\pi\sigma^{2},$$

which, together with (*), implies that

$$\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\sigma^2}x^2\right) dx = I = (2\pi\sigma^2)^{1/2}.$$

Finally, by further substituting $x = z - \mu$, we have

$$1 = \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{(z-\mu)^2}{2\sigma^2}\right) dz$$
$$= \int_{-\infty}^{\infty} \mathcal{N}(z|\mu, \sigma^2) dz.$$

(1.49)

$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x \, \mathrm{d}x$$
$$= \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) x \, \mathrm{d}x.$$

Applying the transformation $z = x - \mu$, we obtain

$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{z^2}{2\sigma^2}\right) (z+\mu) \, \mathrm{d}z$$

$$= \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{z^2}{2\sigma^2}\right) z \, \mathrm{d}z + \mu \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{z^2}{2\sigma^2}\right) \, \mathrm{d}z$$

$$= \mu,$$

where in the second last step, the first term vanishes because it integrates over an odd function.

(1.50)

Recall

$$\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) \, \mathrm{d}x = 1.$$

Differentiating both sides with respect to σ^2 , we have

$$\begin{split} 0 &= \frac{\partial}{\partial \sigma^2} \int_{-\infty}^{\infty} \mathcal{N}(x|\mu,\sigma^2) \, \mathrm{d}x \\ &= -\int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\bigg(-\frac{(x-\mu)^2}{2\sigma^2} \bigg) \frac{(\sigma^2)^{-1}}{2} \, \mathrm{d}x + \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\bigg(-\frac{(x-\mu)^2}{2\sigma^2} \bigg) \frac{(x-\mu)^2(\sigma^2)^{-2}}{2} \, \mathrm{d}x \\ &= -\frac{1}{2} \int_{-\infty}^{\infty} \mathcal{N}(x|\mu,\sigma^2)(\sigma^2)^{-1} \, \mathrm{d}x + \frac{1}{2} \int_{-\infty}^{\infty} \mathcal{N}(x|\mu,\sigma^2)(x-\mu)^2(\sigma^2)^{-2} \, \mathrm{d}x. \end{split}$$

Multiplying $2\sigma^4$ on both sides, we obtain

$$0 = -\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) \sigma^2 \, \mathrm{d}x + \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) (x - \mu)^2 \, \mathrm{d}x$$

$$= -\sigma^2 \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) \, \mathrm{d}x + \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x^2 \, \mathrm{d}x - 2\mu \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x \, \mathrm{d}x + \mu^2 \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) \, \mathrm{d}x$$

$$= -\sigma^2 + \mathbb{E}[x^2] - 2\mu \mathbb{E}[x] + \mu^2$$

$$= -\sigma^2 + \mathbb{E}[x^2] - \mu^2.$$

Therefore, $\mathbb{E}[x^2] = \mu^2 + \sigma^2$.

(1.51)

Combining (1.49) and (1.50), it is easy to see that

$$var[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2.$$

(1.55)

Recall the log likelihood function

$$\ell(\mu, \sigma) = -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu)^2 - \frac{N}{2} \ln \sigma^2 - \frac{N}{2} \ln(2\pi).$$

Solving for $\mu_{\rm ML}$, we obtain

$$\mu_{\text{ML}} = \arg_{\mu} \left(\frac{\partial}{\partial \mu} \ell(\mu, \sigma) = 0 \right) \Big|_{\sigma^2 = \sigma_{\text{ML}}^2}$$
$$= \arg_{\mu} \left(\frac{1}{\sigma^2} \sum_{n=1}^{N} (x_n - \mu) = 0 \right)$$
$$= \frac{1}{N} \sum_{n=1}^{N} x_n.$$

(1.56)

$$\sigma_{\text{ML}}^2 = \arg_{\sigma^2} \left(\frac{\partial}{\partial \sigma^2} \ell(\mu, \sigma) = 0 \right) \Big|_{\mu = \mu_{\text{ML}}}$$

$$= \arg_{\sigma^2} \left(\frac{1}{2} \sum_{n=1}^N (x_n - \mu_{\text{ML}})^2 (\sigma^2)^{-2} - \frac{N}{2} \frac{1}{\sigma^2} = 0 \right)$$

$$= \frac{1}{N} \sum_{n=1}^N (x_n - \mu_{\text{ML}})^2.$$

(1.57)

$$\mathbb{E}[\mu_{\text{ML}}] = \mathbb{E}\left[\frac{1}{N} \sum_{n=1}^{N} x_n\right]$$
$$= \frac{1}{N} \mathbb{E}\left[\sum_{n=1}^{N} x_n\right]$$
$$= \frac{1}{N} N \mu$$
$$= \mu,$$

where the third step took advantage of the fact that the data points are independent, identically distributed, so that $\mathbb{E}[x_n] = \mu$ for any $n \in \{1, \dots, N\}$.

(1.58)

$$\mathbb{E}[\sigma_{\text{ML}}^{2}] = \mathbb{E}\left[\frac{1}{N}\sum_{n=1}^{N}(x_{n} - \mu_{\text{ML}})^{2}\right]$$

$$= \mathbb{E}\left[\frac{1}{N}\sum_{n=1}^{N}(x_{n} - \frac{1}{N}\sum_{m=1}^{N}x_{m})^{2}\right]$$

$$= \frac{1}{N}\mathbb{E}\left[\sum_{n=1}^{N}x_{n}^{2} - \frac{2}{N}\left(\sum_{n=1}^{N}x_{n}\right)^{2} + \frac{1}{N^{2}}\sum_{n=1}^{N}\left(\sum_{m=1}^{N}x_{m}\right)^{2}\right]$$

$$= \frac{1}{N}\mathbb{E}\left[\sum_{n=1}^{N}x_{n}^{2}\right] - \frac{2}{N^{2}}\mathbb{E}\left[\left(\sum_{n=1}^{N}x_{n}\right)^{2}\right] + \frac{1}{N^{3}}\mathbb{E}\left[\sum_{n=1}^{N}\left(\sum_{m=1}^{N}x_{m}\right)^{2}\right]$$

$$= \frac{1}{N}\mathbb{E}\left[\sum_{n=1}^{N}x_{n}^{2}\right] - \frac{2}{N^{2}}\mathbb{E}\left[\left(\sum_{n=1}^{N}x_{n}\right)^{2}\right] + \frac{1}{N^{2}}\mathbb{E}\left[\left(\sum_{m=1}^{N}x_{m}\right)^{2}\right]$$

$$= \frac{1}{N}\mathbb{E}\left[\sum_{n=1}^{N}x_{n}^{2}\right] - \frac{1}{N^{2}}\mathbb{E}\left[\left(\sum_{n=1}^{N}x_{n}\right)^{2}\right]$$

$$= \frac{1}{N}N(\mu^{2} + \sigma^{2}) - \frac{1}{N^{2}}(N^{2}\mu^{2} + N\sigma^{2})$$

$$= \frac{N-1}{N}\sigma^{2}.$$

In the second last step, for the first term, analogous to the proof of (1.57), we made use of the i.i.d. assumption such that $\mathbb{E}[x_n^2] = \mu^2$ for any $n \in \{1, \dots, N\}$. In terms of the second term, for any $m, n \in \{1, \dots, N\}$, we have $\mathbb{E}[x_n x_m] = \mu^2 + I_{nm} \sigma^2$, where $I_{nm} = 1$ if n = m, and $I_{nm} = 0$ otherwise. If we expand the square of sum, there are N out of N^2 terms with n = m, and $N^2 - N$ terms with $n \neq m$, which gives rise to the result.

1.5 Decision Theory

(1.88)

Let

$$G(y, \mathbf{x}) = \int \{y(\mathbf{x}) - t\}^2 p(\mathbf{x}, t) dt,$$

such that

$$\mathbb{E}[L] = \int G(y, \mathbf{x}) \, \mathrm{d}\mathbf{x}.$$

Using Euler-Lagrange equation, we obtain

$$\frac{\partial G(y, \mathbf{x})}{\partial y(\mathbf{x})} = 2 \int \{y(\mathbf{x}) - t\} p(\mathbf{x}, t) \, dt = 0.$$

(1.90)

$$\mathbb{E}[L] = \iint \{y(\mathbf{x}) - t\}^2 p(\mathbf{x}, t) \, d\mathbf{x} \, dt$$

$$= \iint \{y(\mathbf{x}) - \mathbb{E}_t[t|\mathbf{x}] + \mathbb{E}_t[t|\mathbf{x}] - t\}^2 p(\mathbf{x}, t) \, d\mathbf{x} \, dt$$

$$= \iint \left\{ (y(\mathbf{x}) - \mathbb{E}_t[t|\mathbf{x}])^2 + 2(y(\mathbf{x}) - \mathbb{E}_t[t|\mathbf{x}])(\mathbb{E}_t[t|\mathbf{x}] - t) + (\mathbb{E}_t[t|\mathbf{x}] - t)^2 \right\} p(\mathbf{x}, t) \, d\mathbf{x} \, dt$$

$$= \iint (y(\mathbf{x}) - \mathbb{E}_t[t|\mathbf{x}])^2 p(\mathbf{x}, t) \, d\mathbf{x} \, dt + \iint (\mathbb{E}_t[t|\mathbf{x}] - t)^2 p(\mathbf{x}, t) \, d\mathbf{x} \, dt +$$

$$2 \iint (y(\mathbf{x}) - \mathbb{E}_t[t|\mathbf{x}])(\mathbb{E}_t[t|\mathbf{x}] - t) p(\mathbf{x}, t) \, d\mathbf{x} \, dt.$$

Expanding the third term while omitting the coefficient 2, we have

$$\iint (y(\mathbf{x}) - \mathbb{E}_t[t|\mathbf{x}])(\mathbb{E}_t[t|\mathbf{x}] - t)p(\mathbf{x}, t) \, d\mathbf{x} \, dt \\
= \iint y(\mathbf{x})\mathbb{E}_t[t|\mathbf{x}]p(\mathbf{x}, t) \, d\mathbf{x} \, dt - \iint y(\mathbf{x})tp(\mathbf{x}, t) \, d\mathbf{x} \, dt - \iint \mathbb{E}_t[t|\mathbf{x}]^2p(\mathbf{x}, t) \, d\mathbf{x} \, dt + \iint \mathbb{E}_t[t|\mathbf{x}]tp(\mathbf{x}, t) \, d\mathbf{x} \, dt \\
= \mathbb{E}_t[t|\mathbf{x}] \int y(\mathbf{x}) \int p(\mathbf{x}, t) \, dt \, d\mathbf{x} - \int y(\mathbf{x})p(\mathbf{x}) \int tp(t|\mathbf{x}) \, dt \, d\mathbf{x} - \mathbb{E}_t[t|\mathbf{x}]^2 + \mathbb{E}_t[t|\mathbf{x}] \int tp(t|\mathbf{x}) \int p(\mathbf{x}) \, d\mathbf{x} \, dt \\
= \mathbb{E}_t[t|\mathbf{x}]\mathbb{E}_y[\mathbf{x}] - \mathbb{E}_t[t|\mathbf{x}]\mathbb{E}_y[\mathbf{x}] - \mathbb{E}_t[t|\mathbf{x}]^2 + \mathbb{E}_t[t|\mathbf{x}]^2 \\
= 0.$$

Thus, the cross term vanishes and we obtain

$$\mathbb{E}[L] = \iint (y(\mathbf{x}) - \mathbb{E}_t[t|\mathbf{x}])^2 p(\mathbf{x}, t) \, d\mathbf{x} \, dt + \iint (\mathbb{E}_t[t|\mathbf{x}] - t)^2 p(\mathbf{x}, t) \, d\mathbf{x} \, dt$$

$$= \iint (y(\mathbf{x}) - \mathbb{E}_t[t|\mathbf{x}])^2 \int p(t|\mathbf{x}) \, dt \, d\mathbf{x} + \iint (\mathbb{E}_t[t|\mathbf{x}] - t)^2 p(\mathbf{x}, t) \, d\mathbf{x} \, dt$$

$$= \iint (y(\mathbf{x}) - \mathbb{E}_t[t|\mathbf{x}])^2 \, d\mathbf{x} + \iint (\mathbb{E}_t[t|\mathbf{x}] - t)^2 p(\mathbf{x}, t) \, d\mathbf{x} \, dt.$$

Note that this result is different from the one in the book.