

Chapter 1 Introduction

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1.2 Probability Theory

(1.27)

For the transformation $x = g(y)$, the "volume" of x is changed by the determinant of the Jacobian matrix, that is

$$dy = \left| \frac{dy}{dx} \right| dx.$$

Since the probability density integrates to one, this change must be balanced out from the density function, which is given by

$$p_y(y) = p_x(x) \left| \frac{dx}{dy} \right|,$$

such that

$$\begin{aligned} \int p_x(x) dx &= \int \underbrace{p_x(x) \left| \frac{dx}{dy} \right|}_{p_y(y)} \underbrace{\left| \frac{dy}{dx} \right|}_{dy} dx \\ &= \int p_y(y) dy. \end{aligned}$$

Therefore,

$$\begin{aligned} p_y(y) &= p_x(x) \left| \frac{dx}{dy} \right| \\ &= p_x(g(y)) |g'(y)|. \end{aligned}$$

(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

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

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), the above equation can be reduced to

$$\begin{aligned} I^2 &= \int_0^{2\pi} \int_0^\infty \exp\left(-\frac{1}{2\sigma^2}(r \cos \theta)^2 - \frac{1}{2\sigma^2}(r \sin \theta)^2\right) \left| \frac{\partial(x, y)}{\partial(r, \theta)} \right| dr d\theta \\ &= \int_0^{2\pi} \int_0^\infty \exp\left(-\frac{r^2}{2\sigma^2}\right) r dr d\theta. \end{aligned}$$

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

$$\begin{aligned} I^2 &= \int_0^{2\pi} \int_0^\infty \exp\left(-\frac{u}{2\sigma^2}\right) u^{1/2} \left| \frac{dr}{du} \right| du d\theta \\ &= \int_0^{2\pi} \int_0^\infty \frac{1}{2} \exp\left(-\frac{u}{2\sigma^2}\right) du d\theta \\ &= -\sigma^2 \exp\left(-\frac{u}{2\sigma^2}\right) \Big|_0^\infty \int_0^{2\pi} d\theta \\ &= 2\pi\sigma^2, \end{aligned}$$

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 making another substitution $x = z - \mu$, we have

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

(1.49)

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

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

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

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

(1.50)

Recall the normalization condition of the Gaussian distribution

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

differentiating on both sides w.r.t. σ^2 , we have

$$\begin{aligned}
0 &= \frac{\partial}{\partial \sigma^2} \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx \\
&= - \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \frac{(\sigma^2)^{-1}}{2} dx + \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \frac{(x-\mu)^2(\sigma^2)^{-2}}{2} dx \\
&= -\frac{1}{2} \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) (\sigma^2)^{-1} dx + \frac{1}{2} \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) (x-\mu)^2 (\sigma^2)^{-2} dx,
\end{aligned}$$

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

$$\begin{aligned}
0 &= - \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) \sigma^2 dx + \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) (x-\mu)^2 dx \\
&= -\sigma^2 \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx + \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x^2 dx - 2\mu \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x dx + \mu^2 \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx \\
&= -\sigma^2 + \mathbb{E}[x^2] - 2\mu\mathbb{E}[x] + \mu^2 \\
&= -\sigma^2 + \mathbb{E}[x^2] - \mu^2.
\end{aligned}$$

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

(1.51)

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

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

(1.55)

Recall the log likelihood function

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

μ_{ML} can be computed by

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

(1.56)

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

(1.57)

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

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

(1.58)

$$\begin{aligned}
\mathbb{E}[\sigma_{\text{ML}}^2] &= \mathbb{E}\left[\frac{1}{N} \sum_{n=1}^N (x_n - \mu_{\text{ML}})^2\right] \\
&= \mathbb{E}\left[\frac{1}{N} \sum_{n=1}^N (x_n - \frac{1}{N} \sum_{m=1}^N x_m)^2\right] \\
&= \frac{1}{N} \mathbb{E}\left[\sum_{n=1}^N x_n^2 - \frac{2}{N} \left(\sum_{n=1}^N x_n\right)^2 + \frac{1}{N^2} \sum_{n=1}^N \left(\sum_{m=1}^N x_m\right)^2\right] \\
&= \frac{1}{N} \mathbb{E}\left[\sum_{n=1}^N x_n^2\right] - \frac{2}{N^2} \mathbb{E}\left[\left(\sum_{n=1}^N x_n\right)^2\right] + \frac{1}{N^3} \mathbb{E}\left[\sum_{n=1}^N \left(\sum_{m=1}^N x_m\right)^2\right] \\
&= \frac{1}{N} \mathbb{E}\left[\sum_{n=1}^N x_n^2\right] - \frac{2}{N^2} \mathbb{E}\left[\left(\sum_{n=1}^N x_n\right)^2\right] + \frac{1}{N^2} \mathbb{E}\left[\left(\sum_{m=1}^N x_m\right)^2\right] \\
&= \frac{1}{N} \mathbb{E}\left[\sum_{n=1}^N x_n^2\right] - \frac{1}{N^2} \mathbb{E}\left[\left(\sum_{n=1}^N x_n\right)^2\right] \\
&= \frac{1}{N} N(\mu^2 + \sigma^2) - \frac{1}{N^2} (N^2 \mu^2 + N\sigma^2) \\
&= \frac{N-1}{N} \sigma^2.
\end{aligned}$$

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

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

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)

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

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

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

Thus, the cross term vanishes and we obtain

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

This result is different from (1.90) in the textbook.