21. Variation in rat pupil area. Implied distributions and integration by substitution

Pairs of random variables can be related deterministically even if their distributions are quite different. For example, Figure 1(a) shows a possible p.d.f. for the distribution of pupil radius, R, in rats; see Appendix 21 for details. The mode of this distribution is 0.5 mm. Figure 1(b) shows the corresponding p.d.f. for pupil area, A. The mode is now zero, i.e., the distribution is no longer bell-shaped. Thus the two random variables R and A have quite different distributions. Nevertheless, for any given rat, R and A are related deterministically by $A = \pi R^2$.

Because of this deterministic relationship between radius and area, there are two different ways to calculate size probabilities for rat pupils. Suppose, e.g., you require the probability that a randomly chosen pupil radius lies between 0.5 and 0.75 mm. Then you could calculate Prob($0.5 \le R \le 0.75$) directly from the distribution of R. On the other hand, observing that radius lies between 0.5 and 0.75 if and only if area lies between 0.25π and 0.5625π, you could instead calculate Prob($0.25\pi \le A \le 0.5625\pi$) from the distribution of A. Your answers would have to be the same, because there is a fixed probability of a certain size of pupil for a randomly chosen rat. The distribution of R must therefore imply the distribution of A, and vice versa. Here we reveal how.

Let F and f be the c.d.f. and p.d.f for radius, and let G and g be the corresponding c.d.f. and p.d.f for area. Thus

$$F(x) \;=\; \text{Prob}(R \le x) \;=\; \int_0^x f(t)dt \qquad (21.1)$$

is the probability that radius does not exceed x, and

$$G(u) \;=\; \text{Prob}(A \le u) \;=\; \int_0^u g(t)dt \qquad (21.2)$$

is the probability that area does not exceed u. Because radius and area are nonnegative, $R \le x$ if and only if $\pi R^2 \le \pi x^2$. So $F(x) = \text{Prob}(R \le x) = \text{Prob}(\pi R^2 \le \pi x^2) = \text{Prob}(A \le \pi x^2)$ $= G(\pi x^2)$, by (2). That is,

$$F(x) \;=\; G(\pi x^2). \qquad (21.3)$$

Hence, by the chain rule,

$$F'(x) \;=\; G'(\pi x^2)\frac{d\{\pi x^2\}}{dx} \;=\; G'(\pi x^2)\cdot 2\pi x; \qquad (21.4)$$

and so, by the fundamental theorem of continuous distributions,

$$f(x) \;=\; g(\pi x^2)\cdot 2\pi x. \qquad (21.5)$$

If we replace πx^2 by u, equivalent to replacing x by $\sqrt{u/\pi}$, then (5) reduces to $f(\sqrt{u/\pi})$ $= g(u)\cdot 2\sqrt{u\pi}$. That is, the probability density functions of R and A are related by

$$f(x) \;=\; 2\pi x\, g(\pi x^2) \qquad (21.6a)$$

$$g(u) \;=\; \frac{1}{2\sqrt{\pi u}} f(\sqrt{u/\pi}) \qquad (21.6b)$$

We now apply this result to Figure 1. From Appendix 21 and (20.34)-(20.35), variation in pupil radius is modelled by a Weibull distribution with shape parameter 2, scale parameter $s = 0.713$ and hence mode $s/\sqrt{2} \approx 0.5$ mm. With this value of s in (20.33)-(20.34), the c.d.f. and p.d.f are given by

$$F(x) = 1 - \frac{1}{\exp(\{x/s\}^2)}, \tag{21.7}$$

and

$$f(x) = F'(x) = \frac{2x}{s^2 \exp(\{x/s\}^2)}. \tag{21.8}$$

The probability that radius lies between 0.5 and 0.75 can be calculated directly as

$$\begin{aligned} \mathrm{Prob}(0.5 \le R \le 0.75) &= \int_{0.5}^{0.75} f(x)\,dx \\ &= F(0.75) - F(0.5) \qquad (21.9) \\ &= \frac{1}{\exp(\{0.5/s\}^2)} - \frac{1}{\exp(\{0.75/s\}^2)} = 0.2808. \end{aligned}$$

On the other hand, from (6b) and (8), the p.d.f. for pupil area satisfies

$$g(u) = \frac{1}{2\sqrt{\pi u}} \frac{2\sqrt{u/\pi}}{s^2 \exp(\{\sqrt{u}/s\sqrt{\pi}\}^2)} = \frac{1}{\pi s^2 \exp(u/\pi s^2)}. \tag{21.10}$$

Replacing s by πs^2 and m by 1 in (20.34), we see that area has a Weibull distribution with shape parameter 1 and scale parameter πs^2; and, from (20.33), the c.d.f is

$$G(u) = 1 - \frac{1}{\exp(u/\pi s^2)}, \tag{21.11}$$

Thus the probability that radius lies between 0.5 and 0.75 can also be calculated as

$$\begin{aligned} \mathrm{Prob}(0.25\pi \le A \le 0.5625\pi) &= \int_{0.25\pi}^{0.5625\pi} g(u)\,du \\ &= G(0.5625\pi) - G(0.25) \qquad (21.12) \\ &= \frac{1}{\exp(0.25/s^2)} - \frac{1}{\exp(0.5625/s^2)} = 0.2815. \end{aligned}$$

The important point is that

$$\int_{0.5}^{0.75} f(x)\,dx = \int_{0.25\pi}^{0.5625\pi} g(u)\,du \tag{21.13}$$

because both integrals represent exactly the same probability (albeit calculated from different distributions).

More generally, suppose that two random variables R and A (not necessarily radius and area) with distribution functions F, G and density functions f, g are related by $A = \phi(R)$, where ϕ is strictly increasing, and therefore invertible. Let the inverse function be ζ. That is, $A = \phi(R)$ is exactly the same thing as $R = \zeta(A)$, and vice versa; for example, in the special case of rat pupil radius, we have $A = \phi(R) = \pi R^2$ and $R = \zeta(A)$ $= \sqrt{A/\pi}$. Then, because ϕ is strictly increasing, R lies between a and b if and only $\phi(R)$ lies between $\phi(a)$ and $\phi(b)$. So

$$\mathrm{Prob}(a \le R \le b) = F(b) - F(a) = \int_a^b f(x)\,dx \tag{21.14}$$

is identical to

$$\text{Prob}(\phi(a) \le A \le \phi(b)) = G(\phi(b)) - G(\phi(a)) = \int_{\phi(a)}^{\phi(b)} g(u)\,du, \tag{21.15}$$

implying

$$\int_a^b f(x)\,dx = \int_{\phi(a)}^{\phi(b)} g(u)\,du. \tag{21.16}$$

This observation is the key to a more general method for transforming integrals, called **integration by substitution**. In the rat example, the substitution is $u = \pi x^2$. More generally, however, it has the form $u = \phi(x)$ where ϕ is strictly increasing with inverse ζ. Then the **inverse substitution** is $x = \zeta(u)$. Note that ζ is also strictly increasing.[1]

Because ϕ is increasing, $R \le x$ if and only if $\phi(R) \le \phi(x)$. Thus $F(x) = \text{Prob}(R \le x) = \text{Prob}(\phi(R) \le \phi(x)) = \text{Prob}(A \le \phi(x)) = G(\phi(x))$, or

$$F(x) = G(\phi(x)). \tag{21.17}$$

The inverse substitution yields

$$F(\zeta(u)) = G(u). \tag{21.18}$$

Hence, by the chain rule,

$$F'(\zeta(u)) \cdot \zeta'(u) = G'(u) \tag{21.19}$$

and, by the fundamental theorem of continuous distributions,

$$f(\zeta(u)) \cdot \zeta'(u) = g(u). \tag{21.20}$$

Combining (16) and (20), we have our required formula for integration by substitution:

$$\int_a^b f(x)\,dx = \int_{\phi(a)}^{\phi(b)} f(\zeta(u))\,\zeta'(u)\,du \tag{21.21}$$

Note that an inverse functional relationship to (20) is readily found; see Exercise 1.

To illustrate the use of (21), suppose that size not exceeding 1 for some trait is thought to have a (conditional) distribution of the form

$$f(x) = \alpha x(x^2+1)^4, \qquad 0 \le x \le 1. \tag{21.22}$$

where α is a parameter. What must be the value of α? Because total probability is 1,

$$\int_0^1 f(x)\,dx = \int_0^1 \alpha x(x^2+1)^4\,dx = \alpha \int_0^1 x(x^2+1)^4\,dx = 1. \tag{21.23}$$

So $\alpha = 1/I$, where

$$I = \int_0^1 x(x^2+1)^4\,dx. \tag{21.24}$$

To evaluate I, we substitute $u = 1 + x^2$, implying $\phi(x) = 1 + x^2$; hence $x = (u-1)^{1/2}$, implying $\zeta(u) = (u-1)^{1/2}$. The chain rule yields $\zeta'(u) = (u-1)^{-1/2}/2$.[2] Now, from (21) with $a = 0$, $b = 1$ and $f(x) = x(x^2+1)^4$, we have

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[1] The method is readily extended to the case where ϕ is strictly decreasing (Exercise 1), the important point being that ϕ must be invertible.

[2] A slight subtlety here is that, strictly, $\zeta'(u)$ is defined only on (1, 2] because $\zeta'(1+)$ $\zeta'(u)$ approaches ∞ as u approaches 1 from above

$$\begin{aligned} I &= \int_0^1 x(x^2+1)^4\,dx \\ &= \int_{\phi(0)}^{\phi(1)} \zeta(u)\{\zeta(u)^2+1\}^4\zeta'(u)\,du \\ &= \int_1^2 (u-1)^{1/2}u^4(u-1)^{-1/2}/2\,du \qquad (21.25) \\ &= \frac{1}{2}\int_1^2 u^4\,du \;=\; \frac{1}{10}u^5\Big|_1^2 \;=\; \frac{1}{10}\{2^5-1^5\} \;=\; \frac{31}{10} \end{aligned}$$

So $\alpha = 10/31 = 0.3226$.

Integration by substitution is of relatively little importance as a practical method for evaluating specific integrals, which are usually found as readily by other means; for example, (24) can be evaluated by noting that $(x^2+1)^4 = 1+4x^2+6x^4+4x^3+x^8$ implies

$$\begin{aligned} I &= \int_0^1 x(1+4x^2+6x^4+4x^6+x^8)\,dx \;=\; \int_0^1 (x+4x^3+6x^5+4x^7+x^9)\,dx \qquad (21.26) \\ &= \left\{\tfrac{1}{2}x^2+x^4+x^6+\tfrac{1}{2}x^8+\tfrac{1}{10}x^{10}\right\}\Big|_0^1 \;=\; \tfrac{1}{2}+1+1+\tfrac{1}{2}+\tfrac{1}{10} \;=\; \tfrac{31}{10}. \end{aligned}$$

Integration by substitution remains important for theoretical developments, however, and we will make good use of it in the following lecture.

Exercises 21

21.1 (i) Show that the inverse relationship to (20) is $f(x) = g(\phi(x))\cdot\phi'(x)$.

(ii) Obtain (21) in the case where ϕ is strictly decreasing.

21.2 Use the substitution $u=\sqrt{x-1}$ to evaluate $\int_1^5 x\sqrt{x-1}\,dx$.

21.3 Use the substitution $u=\sqrt{x^2-1}$ to evaluate $\int_1^{\sqrt{5}} x^3\sqrt{x^2-1}\,dx$.

21.4 Use the substitution $u=\sqrt{x-1}$ to evaluate

(i) $\int_1^2 (x+2)\sqrt{x-1}\,dx$ (ii) $\int_1^2 (2x+1)\sqrt{x-1}\,dx$

21.5 (i) A function ζ is defined on [0, 15] by $\zeta(u) = u(16-u)^{-1}$. Use the product rule and the chain rule to find an expression for $\zeta'(u)$.

(ii) Use the substitution $u = 16x/(1+x)$ to show that

$$\int_0^{\frac{1}{63}} \frac{64\sqrt{x}}{(1+x)^{7/2}}\,dx = \frac{317}{3840}.$$

Appendix 21

The distributions in Figure 1 model data provided by Dr. Williams. These data were obtained from an experiment with 22 lightly anaesthetized, pigmented (dark-eyed) rats. One at a time, the rats were placed under a low-power microscope and exposed to a given intensity of light (not relevant to our purpose). Each diameter was measured to the nearest 0.25 mm by holding a millimeter scale up to the eye. The results were as shown in Table 1. Because, e.g., any diameter between 0.875 and 1.125mm would be recorded as 1.0, we take Prob($0.875 \le 2R \le 1.125$) = 7/22 or Prob($0.4375 \le R \le 0.5625$) = 7/22, and so on for other radii. We thus obtain the discrete c.d.f. for radius given by Table 2, i.e., $P_n = \text{Prob}(R \le r_n\}$ with $\{r_0, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8\}$ = {0.1875, 0.3125, 0.4375, 0.5625, 0.8125, 1.0625, 1.3125, 1.5625, 1.8125}. This c.d.f. is plotted in Figure 1(c), and the corresponding discrete c.d.f. for area (obtained by squaring each value and multiplying by π) is plotted in Figure 1(d).

DIAMETER	FREQUENCY	DIAMETER	FREQUENCY
0.5 mm	2	2.0 mm	3
0.75 mm	4	2.5 mm	1
1.0 mm	7	3.0 mm	1
1.5 mm	3	3.5 mm	1

Table 21.1 Pupil diameters from an experiment with laboratory rats

RADIUS ≤	PROBABILITY	RADIUS ≤	PROBABILITY
0.3125 mm	1/11	1.0625 mm	19/22
0.4375 mm	3/11	1.3125 mm	10/11
0.5625 mm	13/22	1.5625 mm	21/22
0.8125 mm	8/11	1.8125 mm	1

Table 21.2 Discrete c.d.f. for radius corresponding to Table 1

m	LEAST SUM OF SQUARED ERRORS (Δ)	s AT MINIMUM
1	0.18	0.765
2	0.0349	0.713
3	0.0565	0.655
4	0.0895	0.603

Table 21.3 Least sum of squared errors when fitting (24.33) to rat pupil radius

This c.d.f was fitted to a Weibull distribution (see (20.34)) by the method of Lecture 19. The best-fit shape parameter is m = 2 (see Table 3), and the best-fit scale parameter, i.e., the parameter that minimizes

$$\Delta \;=\; \sum_{n=0}^{8}\left\{1-\frac{1}{\exp(\{r_n/s\}^2)}-P_n\right\}^2, \qquad (21.A1)$$

is s = 0.713. So the c.d.f. of the best-fit continuous distribution is defined on $[0, \infty)$ by

$$F(x) = 1 - \frac{1}{\exp((x/s)^2)} = 1 - \frac{1}{\exp(1.966x^2)}, \qquad (21.A2)$$

and the best-fit p.d.f. by

$$f(x) = F'(x) = \frac{3.932x}{\exp(1.989x^2)}. \qquad (21.A3)$$

Answers and Hints for Selected Exercises

21.1 (ii) See Appendix 22.

21.2 Set I = Int(f, [a, b]) with a = 1, b = 5 and $f(x) = x\sqrt{x-1}$. Then, because $\phi(x) = \sqrt{x-1}$ we have $\phi(a) = \sqrt{1-1} = 0$ and $\phi(b) = \sqrt{5-1} = 2$. Also, $u = \sqrt{x-1}$ implies $u^2 = x - 1 \Rightarrow x = u^2 + 1$. That is, the inverse substitution is defined by $\zeta(u) = u^2 + 1$, implying $\zeta'(u) = 2u$. Now

$$\begin{aligned} I &= \int_a^b f(x)\,dx = \int_{\phi(a)}^{\phi(b)} f(\zeta(u))\,\zeta'(u)\,du \\ &= \int_0^2 \zeta(u)\sqrt{\zeta(u)-1}\,\zeta'(u)\,du = \int_0^2 (u^2+1)\cdot u \cdot 2u\,du \\ &= 2\int_0^2 \{u^2+1\}u^2\,du = 2\int_0^2 \{u^4+u^2\}\,du \\ &= 2\int_0^2 \frac{d}{du}\left\{\frac{u^5}{5}+\frac{u^3}{3}\right\}du = 2\left(\frac{u^5}{5}+\frac{u^3}{3}\right)\Bigg|_0^2 = 2\left(\frac{2^5}{5}+\frac{2^3}{3}-0\right) = \frac{272}{15} \end{aligned}$$

21.3 Set I = Int(f, [a, b]) with a = 1, b = $\sqrt{5}$ and $f(x) = x^3\sqrt{x^2-1}$. Then, because $\phi(x) = \sqrt{x^2-1}$ we have $\phi(a) = \sqrt{a^2-1} = 0$ and $\phi(b) = \sqrt{b^2-1} = 2$. Also, $u = \sqrt{x^2-1} \Rightarrow u^2 = x^2 - 1 \Rightarrow x^2 = u^2+1 \Rightarrow x = \sqrt{u^2+1}$. That is, the inverse substitution is defined by $\zeta(u) = \sqrt{u^2+1} = Q(P(u))$ if Q and P are defined by $P(u) = u^2+1$ and $Q(y) = \sqrt{y} = y^{1/2}$, so that $P'(u) = 2u + 0 = 2u$ and $Q'(y) = \frac{1}{2}y^{-1/2}$. Thus, on using the chain rule, $\zeta'(u) = P'(u)\,Q'(P(u)) = 2u\cdot\frac{1}{2}\{P(u)\}^{-1/2} = u/\sqrt{u^2+1}$. Now

$$\begin{aligned} I &= \int_a^b f(x)\,dx = \int_{\phi(a)}^{\phi(b)} f(\zeta(u))\,\zeta'(u)\,du \\ &= \int_0^2 \zeta(u)^3\sqrt{\zeta(u)^2-1}\,\zeta'(u)\,du = \int_0^2 \left(\sqrt{u^2+1}\right)^3\cdot u\cdot\frac{u}{\sqrt{u^2+1}}\,du \\ &= \int_0^2 \{u^2+1\}u^2\,du = \int_0^2 \{u^4+u^2\}\,du \\ &= \int_0^2 \frac{d}{du}\left\{\frac{u^5}{5}+\frac{u^3}{3}\right\}du = \frac{u^5}{5}+\frac{u^3}{3}\Bigg|_0^2 = \frac{2^5}{5}+\frac{2^3}{3}-0 = \frac{136}{15} \end{aligned}$$

21.4 (i) Set I = Int(f, [a, b]) with a = 1, b = 2 and f(x) = $(x+2)\sqrt{x-1}$. Because ϕ(x) = $\sqrt{x-1}$, we have ϕ(a) = $\sqrt{a-1}$ = 0 and ϕ(b) = $\sqrt{b-1}$ = 2. Also, $u=\sqrt{x-1}$ ⇒ x = u^2+1. That is, the inverse substitution is defined by ζ(u) = u^2+1, so that ζ′(u) = 2u and

$$\begin{aligned} I &= \int_a^b f(x)\,dx = \int_{\phi(a)}^{\phi(b)} f(\zeta(u))\,\zeta'(u)\,du \\ &= \int_0^1 (\zeta(u)+2)\sqrt{\zeta(u)-1}\,\zeta'(u)\,du = \int_0^1 \left(u^2+3\right)\cdot u\cdot 2u\,du \\ &= 2\int_0^1 \{u^2+3\}u^2\,du = 2\int_0^1 \{u^4+3u^2\}\,du \\ &= 2\int_0^1 \frac{d}{du}\left\{\frac{u^5}{5}+u^3\right\}du = 2\left(\frac{u^5}{5}+u^3\right)\Bigg|_0^1 = 2\left(\frac{1^5}{5}+1^3-0\right)\Bigg| = \frac{12}{5} \end{aligned}$$

(ii) Similarly, I = 14/5.

21.5 (i) By the product rule,

$$\zeta'(u) = \frac{d}{du}\{u\}\,(16-u)^{-1} + u\frac{d}{du}\left\{(16-u)^{-1}\right\} = 1\cdot(16-u)^{-1} + u\frac{d}{du}\{Q(P(u))\}$$

if we define Q by Q(y) = y^{-1} and P by P(u) = 16 – u. Then P′(u) = 0 – 1 = -1 and $Q'(y)=-y^{-2}$ (by Table 18.1), implying $Q'(P(u))=-\{P(u)\}^{-2}=-(16-u)^{-2}$. Thus, substituting above and using the chain rule, we have

$$\begin{aligned} \zeta'(u) &= (16-u)^{-1} + uP'(u)Q'(P(u)) \\ &= (16-u)^{-1} + u(-1)\left\{-(16-u)^{-2}\right\} \\ &= \frac{1}{16-u} + \frac{u}{(16-u)^2} = \frac{16}{(16-u)^2}. \end{aligned}$$

Note that we could have avoided using the product rule (but not the chain rule) if we had first observed that ζ(u) = 16/(16–u) – 1.

(ii) Set I = Int(f, [a, b]) with a = 0, b = 1/63 and f(x) = $64\sqrt{x}/(1+x)^{7/2}$. Then, because ϕ(x) = 16x/(1+x) in terms of Lecture 16, we have ϕ(a) = 16a/(1+a) = 0 and ϕ(b) = 16b/(1+b) = 1/4. Also, u = 16x/(1+x) ⇒ u + ux = 16x ⇒ x(16–u) = u ⇒ x = u/(16–u). That is, the inverse substitution is defined by ζ(u) = $u(16-u)^{-1}$. So, from above, ζ′(u) = $16/(16-u)^2$. Now, from (16.21), we have

$$
\begin{aligned}
I \quad &= \quad \int_a^b f(x)\,dx \quad = \quad \int_{\phi(a)}^{\phi(b)} f(\zeta(u))\,\zeta'(u)\,du \\
&= \int_0^{1/4} \frac{64\sqrt{\zeta(u)}}{(1+\zeta(u))^{7/2}} \frac{16}{(16-u)^2}\,du \quad = \quad 4\int_0^{1/4} \frac{16\sqrt{\frac{u}{16-u}}}{\left(1+\frac{u}{16-u}\right)^{7/2}} \frac{16}{(16-u)^2}\,du \\
&= 4\int_0^{1/4} \frac{\sqrt{\frac{u}{16-u}}}{\left(\frac{16}{16-u}\right)^{7/2}} \frac{16^2}{(16-u)^2}\,du \quad = \quad 4\int_0^{1/4} \sqrt{\frac{u}{16-u}} \left(\frac{16-u}{16}\right)^{7/2} \frac{16^2}{(16-u)^2}\,du \\
&= 4\int_0^{1/4} \frac{u^{1/2}}{(16-u)^{1/2}} \left(\frac{16-u}{16}\right)^{3/2}\,du \quad = \quad \frac{4}{16^{3/2}} \int_0^{1/4} u^{1/2}(16-u)\,du \\
&= \frac{1}{16}\int_0^{1/4} \{16u^{1/2} - u^{3/2}\}\,du \quad = \quad \int_0^{1/4} u^{1/2}\,du \quad - \quad \frac{1}{16}\int_0^{1/4} u^{3/2}\,du \\
&= \left.\frac{2u^{3/2}}{3}\right|_0^{\frac{1}{4}} \quad - \quad \frac{1}{16}\cdot\left.\frac{2u^{5/2}}{5}\right|_0^{\frac{1}{4}} \\
&= \frac{2\cdot(1/4)^{3/2}}{3} - \frac{2\cdot 0^{3/2}}{3} \quad - \quad \frac{1}{16}\cdot\left(\frac{2\cdot(1/4)^{5/2}}{5} - \frac{2\cdot 0^{5/2}}{5}\right) \\
&= \frac{1}{12} \quad - \quad \frac{1}{1280} \quad = \quad \frac{317}{3840} \quad (\approx \quad 0.0825521).
\end{aligned}
$$