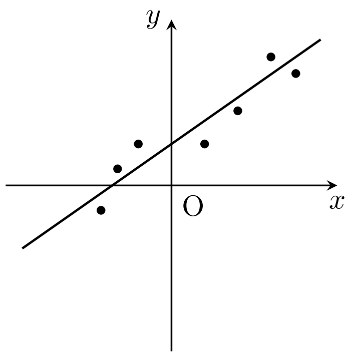
ベイズ推論入門-線形モデル-

2024 年 8 月 8 日

1 問題設定



$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$ から
$y = ax + b$ を求めたい。

$$\begin{cases} a \text{ の確率分布} \\ b \text{ の確率分布} \end{cases}$$

数学的準備

(1) 連立方程式

$$\boldsymbol{y} = A\boldsymbol{x}$$

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$\boldsymbol{x} = A^{-1}\boldsymbol{y}$$

$$A^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

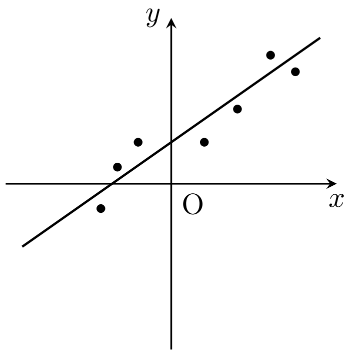
(2) **完全平方**

$$
\begin{aligned}
&ax^2 + bx + c \\
=&a\left\{x^2 + \frac{b}{a}x + \frac{c}{a}\right\} \\
=&a\left\{x^2 + \frac{b}{a}x + \left(\frac{b}{2a}\right)^2 - \left(\frac{b}{2a}\right)^2 + \frac{c}{a}\right\} \\
=&a\left(x + \frac{b}{2a}\right)^2 + a\left(-\frac{b^2}{4a^2}\right) + c \\
=&a\left(x + \frac{b}{2a}\right)^2 - \frac{b^2 - 4ac}{4a}
\end{aligned}
$$

(3) **ガウス分布**

$$
\begin{aligned}
&x\text{：平均 }0\text{，分散 }1 \\
&p(x) = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{x^2}{2}\right) \\
&\int_{-\infty}^{\infty} p(x)dx = 1 \\
☆\quad &z = \sigma x \quad dx = \frac{1}{\sigma}dz \\
&\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}}\frac{dz}{\sigma}\exp\left(-\frac{z^2}{2\sigma^2}\right) = 1 \\
&p(z) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{z^2}{2\sigma^2}\right) \\
☆\quad &y = z + \mu \quad dy = dz \\
&y\text{：平均}\mu\text{，分散}\sigma^2 \\
&\int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right) = 1 \\
&p(y) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right) \\
&y \sim N(\mu, \sigma^2)
\end{aligned}
$$

最小二乗法



$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$ から
$y = ax + b$ を求めたい。

$$\begin{aligned}
E(a,b) &= \frac{1}{N}\sum_{i=1}^{N}\{y_i - (ax_i + b)\}^2 \\
&= \frac{1}{N}\sum_{i=1}^{N}\{y_i^2 - 2y_i(ax_i + b) + (ax_i + b)^2\} \\
&= \frac{1}{N}\sum_{i=1}^{N}\{y_i^2 - 2ax_iy_i - 2by_i + a^2x_i^2 + 2abx_i + b^2\}
\end{aligned}$$

$$\begin{aligned}
\overline{x} &\equiv \frac{1}{N}\sum_{i=1}^{N}x_i \quad \overline{y} \equiv \frac{1}{N}\sum_{i=1}^{N}y_i \\
\overline{x^2} &\equiv \frac{1}{N}\sum_{i=1}^{N}x_i^2 \quad \overline{y^2} \equiv \frac{1}{N}\sum_{i=1}^{N}y_i^2 \\
\overline{xy} &\equiv \frac{1}{N}\sum_{i=1}^{N}x_iy_i
\end{aligned}$$

$$E(a,b) = \overline{y^2} - 2a\overline{xy} - 2b\overline{y} + a^2\overline{x^2} + 2ab\overline{x} + b^2$$

$$\begin{cases}
\frac{\partial E(a,b)}{\partial a} & = -2\overline{xy} + 2a\overline{x^2} + 2b\overline{x} = 0 \\
\frac{\partial E(a,b)}{\partial b} & = -2\overline{y} + 2a\overline{x} + 2b = 0
\end{cases}$$

$$\begin{cases}
a\overline{x^2} + b\overline{x} & = \overline{xy} \\
a\overline{x} + b & = \overline{y}
\end{cases}$$

$$\begin{pmatrix} \overline{x^2} & \overline{x} \\ \overline{x} & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \overline{xy} \\ \overline{y} \end{pmatrix}$$

$$
\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \overline{x^2} & \overline{x} \\ \overline{x} & 1 \end{pmatrix}^{-1} \begin{pmatrix} \overline{xy} \\ \overline{y} \end{pmatrix}
$$

$$
\begin{pmatrix} \overline{x^2} & \overline{x} \\ \overline{x} & 1 \end{pmatrix}^{-1} = \frac{1}{\overline{x^2} - (\overline{x})^2} \begin{pmatrix} 1 & -\overline{x} \\ -\overline{x} & \overline{x^2} \end{pmatrix}
$$

$$
\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\overline{x^2} - (\overline{x})^2} \begin{pmatrix} \overline{xy} - \overline{x}\ \overline{y} \\ \overline{x^2}\ \overline{y} - \overline{x}\ \overline{xy} \end{pmatrix}
$$

$\overline{x} = 0$ としてもよい

$$
E(a,b) = \overline{y^2} - 2a\overline{xy} - 2b\overline{y} + a^2\overline{x^2} + b^2
$$

$$
\frac{\partial E(a,b)}{\partial a} = -2\overline{xy} + 2a\overline{x^2} = 0
$$

$$
a = \frac{\overline{xy}}{\overline{x^2}}
$$

$$
\frac{\partial E(a,b)}{\partial b} = -2\overline{y} + 2b = 0
$$

$$
b = \overline{y}
$$

$$
\begin{pmatrix} \overline{x^2} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \overline{xy} \\ \overline{y} \end{pmatrix}
$$

$$
\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\overline{x^2}} \begin{pmatrix} 1 & 0 \\ 0 & \overline{x^2} \end{pmatrix} \begin{pmatrix} \overline{xy} \\ \overline{y} \end{pmatrix}
$$

$$
\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \overline{xy}/\overline{x^2} \\ \overline{y} \end{pmatrix}
$$

$$
y = ax + b
$$

$$
y_i = ax_i + b
$$

$$
x_i y_i = ax_i^2 + bx_i
$$

$$
\overline{xy} = a\overline{x^2} + b\overline{x}
$$

$$
a = \frac{\overline{xy}}{\overline{x^2}}
$$

$$
\begin{aligned}
E(a,b) &= a^2\overline{x^2} - 2a\overline{xy} + b^2 - 2b\overline{y} + \overline{y^2} \\
&= \overline{x^2}\left(a^2 - 2\frac{\overline{xy}}{\overline{x^2}}a + \left(\frac{\overline{xy}}{\overline{x^2}}\right)^2 - \left(\frac{\overline{xy}}{\overline{x^2}}\right)^2\right) \\
&+ (b^2 - 2b\overline{y} + (\overline{y})^2 - (\overline{y})^2) + \overline{y^2} \\
&= \overline{x^2}\left(a - \frac{\overline{xy}}{\overline{x^2}}\right)^2 + \frac{(\overline{xy})^2}{\overline{x^2}} \\
&+ (b - \overline{y})^2 + \overline{y^2} - (\overline{y})^2 \\
E\left(\frac{\overline{xy}}{\overline{x^2}}, \overline{y}\right) &= \frac{(\overline{xy})^2}{\overline{x^2}} + \overline{y^2} - (\overline{y})^2
\end{aligned}
$$

$$
a_0 = \frac{\overline{xy}}{\overline{x^2}},\ \ b_0 = \overline{y}
$$

$$
E(a,b) = E(a_0, b_0) + \overline{x^2}(a - a_0)^2 + (b - b_0)^2
$$