MODELOWANIE REGRESJI PORZĄDKOWEJ PRZY UŻYCIU PROCESU GAUSSOWSKIEGO

$\{f(x_i)\}_{i=1}^n$ - realizacja procesu gaussowskiego o średniej 0 i macierzy kowariancji $\mathbf{\Sigma}$ zadanej wzorem:

$$\mathbf{\Sigma} = (K(x_i, x_j))_{i,j=1\ldots n} = \left(e^{-\frac{\kappa}{2}\sum_{\xi=1}^d (x_i^\xi - x_i^\xi)^2}\right)_{i,j=1\ldots n},$$

gdzie $\kappa > 0$, a x_i^ξ to ξ-ty element x_i.
Wtedy $\mathbf{f}$ ma rozkład łączny o gęstości:

$$\mathbb{P}(\mathbf{f}) = \frac{1}{Z_f} e^{-\frac{1}{2}\mathbf{f}^T\mathbf{\Sigma}^{-1}\mathbf{f}},$$

gdzie $Z_f = (2\Pi)^{\frac{n}{2}}|\mathbf{\Sigma}|^{\frac{1}{2}}$, a $\mathbf{f} = [f(x_1), \ldots, f(x_n)]^T$.
Wtedy:

$$\mathbb{P}(\mathcal{D}|\mathbf{f}) = \prod_{i=1}^n \mathbb{P}(y_i|f(x_i)),$$

gdzie $\mathcal{D} = \{y_1, \ldots, y_r\}$.
Intuicyjnie:

$$\mathbb{P}_{ideal}(y_i|f(x_i)) = \mathbb{I}\{f(x_i) \in (b_{y_i-1}, b_{y_i}]\},$$

gdzie $b_0 = -\infty, b_r = +\infty$.
Można wygodniej sparametryzować b_i jako: $b_1 \in \mathbb{R}$, $b_i = \sum_{t=2}^j \Delta_t + b_1$, gdzie $\Delta_t > 0$ oraz $j = 2, \ldots, r-1$.
Bardzo rzadko mamy jednak do czynienia z idealną sytuacją, dlatego będziemy budować model zakładając dodatkowy szum δ o rozkładzie $\mathcal{N}(0, \sigma^2)$. Wtedy prawdopodobieństwo zmienia się następująco:

$$\mathbb{P}(y_i|f(x_i)) = \Phi\left(z_1^i\right) - \Phi\left(z_2^i\right),$$

gdzie $z_1^i := \frac{b_{y_i} - f(x_i)}{\sigma}$ oraz $z_2^i := \frac{b_{y_i-1} - f(x_i)}{\sigma}$.

Dowód

$$\mathbb{P}(y_i|f(x_i)) = \int \mathbb{P}_{ideal}(y_i|f(x_i) + \delta_i)d\delta_i = \int \mathbb{P}(\delta_i)\mathbb{I}\{f(x_i) + \delta_i \in (b_{y_i-1}, b_{y_i}]\}d\delta_i =$$
$$= \int \frac{1}{2\Pi\sigma} e^{-\frac{u^2}{2\sigma^2}} \mathbb{I}\{u \in (b_{y_i-1} - f(x_i), b_{y_i} - f(x_i)]\}du = \int_{b_{y_i} - f(x_i)}^{b_{y_i-1} - f(x_i)} \frac{1}{2\Pi\sigma} e^{-\frac{u^2}{2\sigma^2}} du =$$
$$= \int_{\frac{b_{y_i} - f(x_i)}{\delta}}^{\frac{b_{y_i-1} - f(x_i)}{\delta}} \frac{1}{2\Pi} e^{-\frac{u^2}{2}} du = \Phi\left(\frac{b_{y_i} - f(x_i)}{\sigma}\right) - \Phi\left(\frac{b_{y_i-1} - f(x_i)}{\sigma}\right)$$

■

Wprowadźmy następującą funkcję straty:

$$l(y_i, f(x_i)) := -\ln \mathbb{P}(y_i|f(x_i))$$

Jej pochodne to:

$$
\begin{aligned}
\frac{\partial l(y_i, f(x_i))}{\partial f(x_i)} &= \frac{1}{\sigma} \frac{\frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} - \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}}}{\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)} \\
\frac{\partial^2 l(y_i, f(x_i))}{\partial^2 f(x_i)} &= \frac{1}{\sigma^2} \left(\frac{\frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} - \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}}}{\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)} \right)^2 + \frac{1}{\sigma^2} \frac{z_1^i \frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} - z_2^i \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}}}{\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)}
\end{aligned}
$$

Dowód

$$
\begin{aligned}
\frac{\partial l(y_i, f(x_i))}{\partial f(x_i)} &= -\ln\left[\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)\right] = -\frac{1}{\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)} \cdot \Phi'\left(z_1^i\right) \cdot \left(-\frac{1}{\sigma}\right) - \Phi'\left(z_2^i\right) \cdot \left(-\frac{1}{\sigma}\right) = \\
&= \frac{1}{\sigma} \frac{\frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} - \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}}}{\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)} \\
\frac{\partial^2 l(y_i, f(x_i))}{\partial^2 f(x_i)} &= \frac{\partial}{\partial f(x_i)} \left(\frac{\partial l(y_i, f(x_i))}{\partial f(x_i)} \right) = \frac{\partial}{\partial f(x_i)} \left(\frac{1}{\sigma} \frac{\frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} - \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}}}{\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)} \right) = \\
&= \frac{1}{\sigma} \frac{1}{\left[\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)\right]^2} \left\{ \left[\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)\right] \cdot \right. \\
&\cdot \left[\frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} \left(-\frac{1}{\cancel{2}} \cdot \cancel{2}\, z_1^i\right) \left(-\frac{1}{\sigma}\right) - \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}} \left(-\frac{1}{\cancel{2}} \cdot \cancel{2}\, z_2^i\right) \left(-\frac{1}{\sigma}\right) \right] - \\
&- \left. \left(\frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} - \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}} \right) \cdot \left(-\frac{1}{\sigma}\right) \cdot \left(\frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} - \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}} \right) \right\} = \\
&= \frac{1}{\sigma^2} \left(\frac{\frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} - \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}}}{\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)} \right)^2 + \frac{1}{\sigma^2} \frac{z_1^i \frac{1}{2\Pi} e^{-\frac{z_1^{i\,2}}{2}} - z_2^i \frac{1}{2\Pi} e^{-\frac{z_2^{i\,2}}{2}}}{\Phi\left(z_1^i\right) - \Phi\left(z_2^i\right)}
\end{aligned}
$$

■

Prawdopodobieństwo a posteriori wygląda następująco:

$$\mathbb{P}(\mathbf{f}|\mathcal{D}) = \frac{\mathbb{P}(\mathbf{f}) \prod_{i=1}^n \mathbb{P}(y_i|f(x_i))}{\mathbb{P}(\mathcal{D})},$$

gdzie $\mathbb{P}(\mathcal{D}) = \int \mathbb{P}(\mathcal{D}|\mathbf{f})\mathbb{P}(\mathbf{f})d\mathbf{f}$.

Dowód

$$\mathbb{P}(\mathbf{f}|\mathcal{D}) = \frac{\mathbb{P}(\mathbf{f}, \mathcal{D})}{\mathbb{P}(\mathcal{D})} = \frac{\mathbb{P}(\mathcal{D}|\mathbf{f})\mathbb{P}(\mathbf{f})}{\int \mathbb{P}(\mathbf{f}, \mathcal{D})d\mathbf{f}} = \frac{\mathbb{P}(\mathbf{f}) \prod_{i=1}^n \mathbb{P}(y_i|f(x_i))}{\int \mathbb{P}(\mathbf{f}, \mathcal{D})d\mathbf{f}}$$

■

Parametry, które chcemy estymować oznaczmy wektorem $\mathbf{\Theta} = [\kappa, \sigma, b_1, \Delta_2, \ldots, \Delta_{r-1}]^T$.
Szukamy takiego $\mathbf{f}$, które:

$$\mathbf{f}_{MAP} \coloneqq \underset{\mathbf{f}}{\operatorname{argmax}}\{\mathbb{P}(\mathbf{f}|\mathcal{D})\} \equiv \underset{\mathbf{f}}{\operatorname{argmax}}\{\ln \mathbb{P}(\mathbf{f}|\mathcal{D})\} \equiv \underset{\mathbf{f}}{\operatorname{argmin}}\{-\ln \mathbb{P}(\mathbf{f}|\mathcal{D})\}$$

Zdefiniujmy:

$$S(\mathbf{f}) := -\ln \mathbb{P}(\mathbf{f}|\mathcal{D})$$

Wtedy:

$$S(\mathbf{f}) \propto \sum_{i=1}^{n} l(y_i, f(x_i)) + \frac{1}{2}\mathbf{f}^T\mathbf{\Sigma}^{-1}\mathbf{f}$$

Dowód

$$\begin{aligned}
S(f) &= -\ln \mathbb{P}(\mathbf{f}|\mathcal{D}) = -\ln\left[\frac{\mathbb{P}(\mathbf{f})\prod_{i=1}^{n}\mathbb{P}(y_i|f(x_i))}{\mathbb{P}(\mathcal{D})}\right] = -\ln \mathbb{P}(\mathbf{f}) + \ln \mathbb{P}(\mathcal{D}) - \ln\left[\prod_{i=1}^{n}\mathbb{P}(y_i|f(x_i))\right] \propto \\
&\propto -\ln \mathbb{P}(\mathbf{f}) - \ln\left[\prod_{i=1}^{n}\mathbb{P}(y_i|f(x_i))\right] = -\ln\left[\frac{1}{Z_f}e^{-\frac{1}{2}\mathbf{f}^T\mathbf{\Sigma}^{-1}\mathbf{f}}\right] + \sum_{i=1}^{n}\left[-\ln \mathbb{P}(y_i|f(x_i))\right] = \\
&= \frac{1}{2}\mathbf{f}^T\mathbf{\Sigma}^{-1}\mathbf{f} + \ln Z_f + \sum_{i=1}^{n} l(y_i|f(x_i)) \propto \sum_{i=1}^{n} l(y_i|f(x_i)) + \frac{1}{2}\mathbf{f}^T\mathbf{\Sigma}^{-1}\mathbf{f}
\end{aligned}$$

■

Policzmy pochodne $S(f)$:

$$\begin{aligned}
\frac{\partial S(\mathbf{f})}{\partial \mathbf{f}} &= \mathbf{f}^T\mathbf{\Sigma}^{-1} + \left[\frac{\partial l(y_1, f(x_1))}{\partial f(x_1)}, \dots, \frac{\partial l(y_n, f(x_n))}{\partial f(x_n)}\right] \\
\frac{\partial^2 S(\mathbf{f})}{\partial \mathbf{f}\partial \mathbf{f}^T} &= \mathbf{\Sigma}^{-1} + \mathbf{\Lambda},
\end{aligned}$$

gdzie

$$\mathbf{\Lambda} = \begin{bmatrix} \frac{\partial^2 l(y_1, f(x_1))}{\partial^2 f(x_1)} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \frac{\partial^2 l(y_n, f(x_n))}{\partial^2 f(x_n)} \end{bmatrix}$$

Korzystając z przybliżenia Laplace'a otrzymujemy:

$$\mathbb{P}(\mathcal{D}|\mathbf{\Theta}) \simeq e^{-S(\mathbf{f}_{MAP})}\left|\mathbf{I} + \mathbf{\Sigma}\mathbf{\Lambda}_{MAP}\right|^{-\frac{1}{2}},$$

gdzie $\mathbf{I}$ jest macierzą jednostkową $n \times n$.

Dowód

$$
\begin{aligned}
\mathbb{P}(\mathcal{D}|\boldsymbol{\Theta}) &= \int \mathbb{P}(\mathcal{D}|\mathbf{f})\mathbb{P}(\mathbf{f})d\mathbf{f} = \int \frac{1}{Z_f} e^{-\frac{1}{2}\mathbf{f}^T\boldsymbol{\Sigma}^{-1}\mathbf{f}} \prod_{i=1}^{n} \mathbb{P}(y_i|f(x_i))d\mathbf{f} = \\
&= \int \frac{1}{Z_f} e^{-\frac{1}{2}\mathbf{f}^T\boldsymbol{\Sigma}^{-1}\mathbf{f}} e^{\ln\left[\prod_{i=1}^{n} \mathbb{P}(y_i|f(x_i))\right]} d\mathbf{f} = \int \frac{1}{Z_f} e^{-\frac{1}{2}\mathbf{f}^T\boldsymbol{\Sigma}^{-1}\mathbf{f} + \sum_{i=1}^{n}\left[-\ln \mathbb{P}(y_i|f(x_i))\right]} d\mathbf{f} = \\
&= \int \frac{1}{Z_f} e^{-\frac{1}{2}\mathbf{f}^T\boldsymbol{\Sigma}^{-1}\mathbf{f} + \sum_{i=1}^{n} l(y_i|f(x_i))} d\mathbf{f} = \int \frac{1}{Z_f} e^{-S(\mathbf{f})} d\mathbf{f} \overset{\substack{\text{przybliżenie} \\ \text{Laplace'a}}}{\approx} \\
&\approx \frac{1}{Z_f} (2\Pi)^{\frac{n}{2}} \left|\boldsymbol{\Sigma}^{-1} + \boldsymbol{\Lambda}_{MAP}\right|^{-\frac{1}{2}} e^{-S(\mathbf{f}_{MAP})} = \frac{1}{\cancel{(2\Pi)^{\frac{n}{2}}} |\boldsymbol{\Sigma}|^{\frac{1}{2}}} \cancel{(2\Pi)^{\frac{n}{2}}} \left|\boldsymbol{\Sigma}^{-1}(\mathbf{I} + \boldsymbol{\Sigma}\boldsymbol{\Lambda}_{MAP}\right|^{-\frac{1}{2}} e^{-S(\mathbf{f}_{MAP})} = \\
&= \frac{1}{\cancel{|\boldsymbol{\Sigma}|^{\frac{1}{2}}}} \cancel{|\boldsymbol{\Sigma}|^{\frac{1}{2}}} \left|\mathbf{I} + \boldsymbol{\Sigma}\boldsymbol{\Lambda}_{MAP}\right|^{-\frac{1}{2}} e^{-S(\mathbf{f}_{MAP})} = \left|\mathbf{I} + \boldsymbol{\Sigma}\boldsymbol{\Lambda}_{MAP}\right|^{-\frac{1}{2}} e^{-S(\mathbf{f}_{MAP})}
\end{aligned}
$$

■