

1.5.2. Mathematical formulation

1.5.2.1. The initial assumption

1.5.2.2. The best linear unbiased prediction

1.5.2.3. The empirical best linear unbiased predictor

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Initial assumption

- Output

$$g : \mathbb{R}^{n \text{ features}} \rightarrow \mathbb{R}$$

$$X \mapsto y = g(X)$$

- Gaussian process for ML

$$G(X) = \underbrace{f(X)^T \beta}_{\text{線形回帰モデル}} + \underbrace{Z(X)}_{\text{ゼロ平均ガウス過程}}$$

線形回帰モデル



ゼロ平均ガウス過程



$$C(X, X') = \sigma^2 R(|X - X'|)$$

The best linear unbiased prediction

$$\hat{G}(X) = G \left(X \mid y_1 = g(X_1), \dots, y_{n_{\text{samples}}} = g(X_{n_{\text{samples}}}) \right)$$

- 線形性

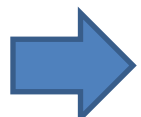
$$\hat{G}(X) \equiv a(X)^T y$$

- 不偏性

$$E[G(X) - \hat{G}(X)] = 0$$

- 最小二乘誤差

$$\hat{G}(X)^* = \arg \min_{\hat{G}(X)} E \left[(G(X) - \hat{G}(X))^2 \right]$$


$$a(X)^* = \arg \min_{a(X)} E \left[(G(X) - a(X)^T y)^2 \right]$$

s. t. $E[G(X) - a(X)^T y] = 0$

The best linear unbiased prediction

- 期待値

$$\mu_{\hat{Y}}(X) = f(X)^T \hat{\beta} + r(X)^T \gamma$$

- 分散

$$\sigma_{\hat{Y}}^2(X) = \sigma_Y^2 (1 - r(X)^T R^{-1} r(X) + u(X)^T (F^T R^{-1} F)^{-1} u(X))$$

$$R_{ij} = R(|X_i - X_j|, \theta), \quad i, j = 1, \dots, m$$

$$r_i = R(|X - X_i|, \theta), \quad i = 1, \dots, m$$

$$F_{ij} = f_i(X_j), \quad i = 1, \dots, p, \quad j = 1, \dots, m$$

$$\hat{\beta} = (F^T R^{-1} F)^{-1} F^T R^{-1} Y$$

$$\gamma = R^{-1} (Y - F \hat{\beta})$$

$$u(X) = F^T R^{-1} r(X) - f(X)$$

} 事前に分からない
モデルを経験的に選択
(EBLUP)