WAIC and WBIC

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(1) $X_1, X_2, \ldots, X_n$, and X … (i.i.d.) … $q(x)\,dx$.

(2) Statistical Model, $p(x|w)$.

(3) Prior, $\varphi(w)$.

(4) Posterior, $p(w|D) = (1/Z(\beta)) \prod_{i=1}^{n} p(X_i|w)^{\beta}\, \varphi(w)$.

Average using posterior $E_w^{\beta}[\ \ ] = \int (\ \ \ )\ p(w|D)\, dw$.

(5) Bayes Marginal, $F = -\log Z(1)$.

(6) Bayes Prediction, $p^*(x) = E_w^{1}[\, p(x|w)\,]$.

(7) Generalization Loss, $G = -\ E_X[\, \log p^*(X)\,]$.

(8) Training Loss, $T = -(1/n) \sum_{i=1}^{n} \log p^*(X_i)$.

(9) Functional Variance,

$$V = \sum_{i=1}^{n} \{\ E_w^{1}[\, (\log p(X_i|w))^2\,] - E_w^{1}[\, \log p(X_i|w)\,]^2\ \}.$$

(10) $\mathrm{WAIC} = T + V/n$.

(11) $\mathrm{WBIC} = -\ E_w^{(1/\log n)}[\ \sum_{i=1}^{n} \log p(X_i|w)\ ]$.

(12) $E[\ \ ]$: The expectation value over $X_1, X_2, \ldots, X_n$.

[Theorem] Even if $q(x)$ is unrealizable by or singular for $p(x|w)$,

$$E[\, G\,] = E[\, \mathrm{WAIC}\,] + O(\tfrac{1}{n^2}),$$

$$F = \mathrm{WBIC} + O_p(\, (\log n)^{1/2}).$$

Relations among Information Criteria

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(1) $L_n(w) = -(1/n) \sum_{i=1}^{n} \log p(X_i|w)$.

(2) $w^* = \mathrm{argmin}\ L_n(w)$ (MLE), $d = \mathrm{dimension}(w)$.

(3) $AIC = L_n(w^*) + d/n$.

(4) $BIC = nL_n(w^*) + (d/2) \log n$.

(5) $DIC = L_n(E_w^1[w]) + (2/n) \{ E_w^1[nL_n(w)] - nL_n(E_w^1[w]) \}$.

(6) $p^{*(-i)}(x)$: Bayes prediction leaving out X_i.

(7) $LOOCV = -(1/n) \sum_{i=1}^{n} \log p^{*(-i)}(X_i)$.

[Theorem] If q(x) is realizable by and regular for p(x|w),

$$WAIC = AIC + o_p\left(\frac{1}{n}\right),$$

$$WAIC = DIC + o_p\left(\frac{1}{n}\right),$$

$$WBIC = BIC + o_p(1).$$

[Theorem] Even if q(x) is unrealizable by or singular for p(x|w),

$$WAIC = LOOCV + O_p\left(\frac{1}{n^2}\right),$$

$$V[WAIC-L_n(w_0)] = V[G-L(w_0)] + o\left(\frac{1}{n^2}\right),$$

$$V[LOOCV-L_n(w_0)] = V[G-L(w_0)] + o\left(\frac{1}{n^2}\right).$$