§2. 判別適合的損失

$R(f) = \mathbb{E}[\mathbb{1}[Y \neq \mathrm{sign}(f(X))]]$ vs. $R_\phi(f) = \mathbb{E}_{(X,Y)}[\phi(Yf(X))]$.

Q. $\forall \mathcal{D} \in \Delta(\mathcal{X} \times \mathcal{Y})$, $\forall (f_m)_{m \in \mathbb{N}} \subseteq \mathcal{M}(\mathcal{X}, \mathbb{R})$

$\forall \varepsilon > 0$ $\exists \delta > 0$ s.t. $R_\phi(f_m) - R_\phi^* < \delta \Rightarrow R(f_m) - R^* < \varepsilon$?

(∃ は具体的に構成.)

- **Def. 適合関数**. ϕ に対して,

$$\delta(\varepsilon) := \inf_{\eta \in [0,1]} \inf_{\alpha \in \mathbb{R}} \left\{ C_{\phi,\eta}(\alpha) - C_{\phi,\eta}^* \;\middle|\; C_\eta(\alpha) - C_\eta^* \geq \varepsilon \right\}.$$

ただし,

条件つき ϕ-リスク	$C_{\phi,\eta}(\alpha)$	$:= \eta\phi(\alpha) + (1-\eta)\phi(-\alpha)$
条件つき Bayes ϕ-リスク	$C_{\phi,\eta}^*$	$:= \inf_{\alpha \in \mathbb{R}} C_{\phi,\eta}(\alpha)$
条件つき 01-リスク	$C_\eta(\alpha)$	$:= \eta\mathbb{1}[\alpha \leq 0] + (1-\eta)\mathbb{1}[\alpha > 0]$.
条件つき Bayes 01-リスク	C_η^*	$:= \inf_{\alpha \in \mathbb{R}} C_\eta(\alpha)$

Remark: α "=" $f(x)$, η "=" $\Pr(Y=1 \mid X=x)$ の気持ち.

特に, $C_{\phi,\eta(x)}(f(x)) = \mathbb{E}_{Y \sim 1|X=x}[\phi(Yf(x))]$.

$$R_\phi(f) = \mathbb{E}_X \mathbb{E}_{Y \sim 1|X=x}[\phi(Yf(x))] = \mathbb{E}_X[C_{\phi,\eta(x)}(f(x))].$$

さらに $R_\phi^* = \inf_{f \in \mathcal{M}(\mathcal{X},\mathbb{R})} \mathbb{E}_{X,Y}[\phi(Yf(x))] \overset{\text{gap}}{=} \mathbb{E}_X\left[\inf_{\alpha \in \mathbb{R}} C_{\phi,\eta(x)}(\alpha)\right] = \mathbb{E}_X[C_{\phi,\eta(x)}^*]$

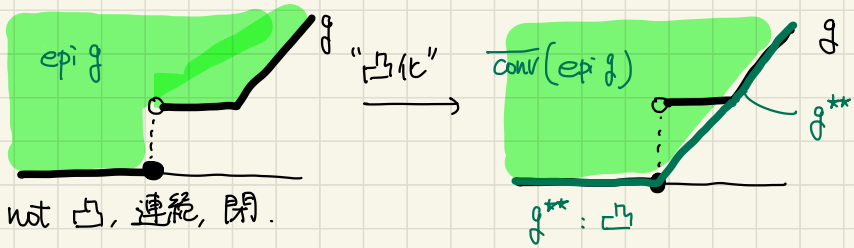
gap (𝔼と inf を交換) ⇝ 講義ページの補足資料参照

- **Def.** $g : \mathbb{R} \to \mathbb{R}$ の **Fenchel 双共役** (biconjugate) $g^{**} : \mathbb{R} \to \mathbb{R}$ を以下で定義:

$$\mathrm{epi}\, g^{**} = \overline{\mathrm{conv}}(\mathrm{epi}\, g)$$

ただし $\mathrm{epi}\, g := \{(x,y) : y \geq g(x)\}$, 凸包 $\mathrm{conv}(S) := \left\{ \sum_{i=1}^m \alpha_i x_i \;\middle|\; \sum_{i=1}^m \alpha_i = 1, \alpha_i \geq 0, x_i \in S \right\}$.

$\overline{\mathrm{conv}}(S)$ は $\mathrm{conv}(S)$ の閉包 (closure)



g: not 凸, 連続, 閉.

Thm 2.1

1) $\forall \mathcal{D} \in \Delta(X,Y)$, $\forall f \in \mathcal{M}(X,\mathbb{R})$,

$$\delta^{**}\left(R(f) - R^*\right) \leq R_\phi(f) - R_\phi^*.$$

2) $\delta(\varepsilon) > 0 \ (\forall \varepsilon > 0)$ のとき $\forall \mathcal{D}$, $(f_m)_{m\geq 1}$ に対し,

$$R_\phi(f_m) \to R_\phi^* \implies R(f_m) \to R^*.$$

この条件を満たす ϕ を**判別適合的**と呼ぶ.
(classification-calibrated.)

Lem 2.2 Bayes rule $f^*(x) := \mathrm{Pr}(Y=1 \mid X=x) - \frac{1}{2}$ によって $R(f^*) = R^*$ が達成

Proof)

$$\begin{aligned} R^* &= \inf_{\uparrow} \mathbb{E}\left[\mathbb{1}[Y \neq \mathrm{sign}(f(X))]\right] \\ &= \mathbb{E}_X\left[\inf_{\alpha\in\mathbb{R}} \eta\,\mathbb{1}[\alpha \leq 0] + (1-\eta)\,\mathbb{1}[\alpha > 0]\right] \qquad ;\ \eta = \mathrm{Pr}(Y=1 \mid X=x) \end{aligned}$$

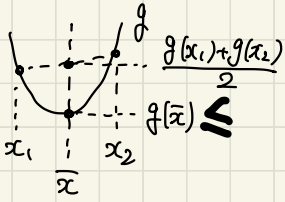
$$\inf_{\alpha\in\mathbb{R}} (2\eta - 1)\,\mathbb{1}[\alpha \leq 0] + (1-\eta).$$

この inf は $\alpha = \eta - \frac{1}{2}$ で達成. □

Remark: $R^* = R(f^*) = \mathbb{E}_X\left[C_\eta(f^*(X))\right] = \mathbb{E}_X\left[C_\eta^*\right]$

- Proof of Thm 2.1)

$$\begin{aligned} \delta^{**}\left(R(f) - R^*\right) &= \delta^{**}\left(\mathbb{E}_X\left[C_\eta(f(X)) - C_\eta^*\right]\right) \\ &\leq \mathbb{E}_X\left[\delta^{**}\left(C_\eta(f(X)) - C_\eta^*\right)\right] \qquad \text{(Jensen)} \\ &\leq \mathbb{E}_X\left[\delta\left(C_\eta(f(X)) - C_\eta^*\right)\right] \end{aligned}$$



δ の定義より　$\delta\left(C_\eta(\alpha) - C_\eta^*\right) \le C_{\phi,\eta}(\alpha) - C_{\phi,\eta}^*$

cf. contraposition 対偶.

$\forall \eta \in [0,1]\ \forall \alpha \in \mathbb{R}$

$\forall \varepsilon > 0.\ \exists \delta > 0$ s.t. $C_\eta(\alpha) - C_\eta^* \ge \varepsilon \Rightarrow C_{\phi,\eta}(\alpha) - C_{\phi,\eta}^* \ge \delta$.

$\Updownarrow$

$C_{\phi,\eta}(\alpha) - C_{\phi,\eta}^* < \delta \Rightarrow C_\eta(\alpha) - C_\eta^* < \varepsilon$.

$\delta(\varepsilon) = \inf_{\eta,\alpha} \left\{ C_{\phi,\eta}(\alpha) - C_{\phi,\eta}^* \mid C_\eta(\alpha) - C_\eta^* \ge \varepsilon \right\}$

$$\begin{aligned}
\delta^{**}(R(f) - R^*) &\le \mathbb{E}_X\left[\delta\left(C_\eta(f(x)) - C_\eta^*\right)\right] \\
&\le \mathbb{E}_X\left[C_{\phi,\eta}(f(x)) - C_{\phi,\eta}^*\right] \\
&= R_\phi(f) - R_\phi^*. \qquad \square
\end{aligned}$$

- 判別適合性の別の表現.

$$\delta(\varepsilon) = \inf_{\eta \in [0,1]} \inf_{\alpha \in \mathbb{R}} \left\{ C_{\phi,\eta}(\alpha) - C_{\phi,\eta}^* \mid \underbrace{C_\eta(\alpha) - C_\eta^* \ge \varepsilon}_{|2\eta-1| \cdot \mathbb{1}\left[\mathrm{sign}(\alpha) \ne \mathrm{sign}\left(\eta - \frac{1}{2}\right)\right]} \right\}.$$

$\mathrm{sign}(\alpha) = \mathrm{sign}\left(\eta - \frac{1}{2}\right)$ のとき：$C_\eta(\alpha) - C_\eta^* \ge \varepsilon$ は常に false.

$\mathrm{sign}(\alpha) \ne \mathrm{sign}\left(\eta - \frac{1}{2}\right)$ のとき：〃 は $|2\eta - 1| \ge \varepsilon$ に成立.

$\Leftrightarrow \eta \le \frac{1-\varepsilon}{2},\ \frac{1+\varepsilon}{2} \le \eta$.

$$= \inf_{\eta \in [0, \frac{1-\varepsilon}{2}] \cup [\frac{1+\varepsilon}{2}, 1]} \underbrace{\left(\inf_{\alpha:\ \mathrm{sign}(\alpha) \ne \mathrm{sign}(\eta - \frac{1}{2})} C_{\phi,\eta}(\alpha) \right)}_{=: C_{\phi,\eta}^-} - C_{\phi,\eta}^*.$$

$$= \inf_{\eta \in [0, \frac{1-\varepsilon}{2}] \cup [\frac{1+\varepsilon}{2}, 1]} \left(C_{\phi,\eta}^- - C_{\phi,\eta}^* \right)$$

$C_{\phi,\eta}^*$: $\forall \alpha \in \mathbb{R}$ での opt.

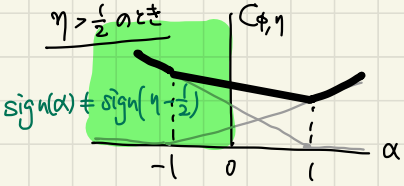
$C_{\phi,\eta}^-$: 誤分類している α での opt.

Fact : ϕ が"判別適合的" $\Leftrightarrow C_{\phi,\eta}^- > C_{\phi,\eta}^*$ $\left(\forall \eta \ne \frac{1}{2}\right)$

- 例1：ヒンジ損失 $\phi(\alpha) = \max\{0, 1-\alpha\} = [1-\alpha]_+$

$C_{\phi,\eta}(\alpha) = \eta[1-\alpha]_+ + (1-\eta)[1+\alpha]_+$

$\eta > \frac{1}{2}$ のとき



$\alpha \in \mathbb{R}$ で inf をとると $\alpha^* = 1$

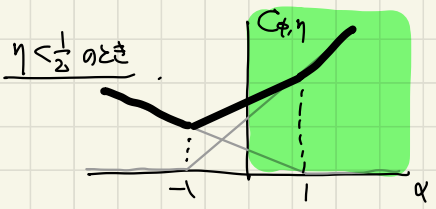
$C^-_{\phi,\eta}$ の inf を実現するのは $\alpha^- = 0$

$\rightsquigarrow C^-_{\phi,\eta} > C^*_{\phi,\eta}$

$\Rightarrow$ ヒンジ損失は 判別適合的.

かつ $\delta(\varepsilon) = \varepsilon$. なので $R(f) - R^* \le R_\phi(f) - R^*_\phi$

$\eta < \frac{1}{2}$ のとき



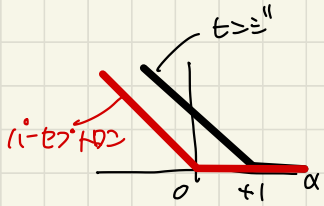
$\alpha^* = -1$

$\alpha^- = 0$

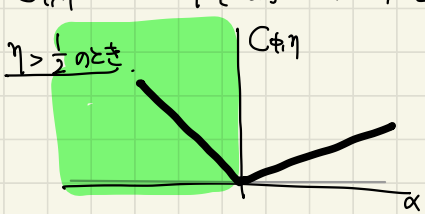
- 例2,3：ロジスティック，二乗損失.

$\Rightarrow$ 判別適合的.

- 反例：パーセプトロン損失 $\phi(\alpha) = [-\alpha]_+$



$C_{\phi,\eta}(\alpha) = \eta[-\alpha] + (1-\eta)[+\alpha]_+$.



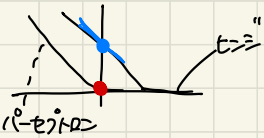
$\alpha^* = 0$, $\alpha^- = 0$ $\rightsquigarrow C^-_{\phi,\eta} = C^*_{\phi,\eta}$ (判別適合的でない)

ちなみに $\delta(\varepsilon) = 0$

- ϕ が凸に限ると 判別適合性の より簡単な表現が得られる.

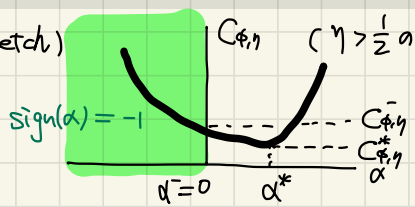
Thm 2.3 ϕ が凸ならば,

ϕ : 判別適合的 $\iff$ ϕ が $\alpha=0$ で可微分 かつ $\phi'(0) < 0$.



Lem 2.4 ϕ が判別適合的であるとき, $C^*_{\phi,\eta} < \phi(0)$ $(\forall \eta \neq \frac{1}{2})$

(proof sketch)



$C^-_{\phi,\eta} = C_{\phi,\eta}(0) = \eta\phi(0) + (1-\eta)\phi(0)$

$= \phi(0)$.

$\vee$

$C^*_{\phi,\eta}$

□