CSE 6740 A/ISyE 6740: Computational Data Analysis: Introductory lecture

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- Overfitting, inductive bias, Intro to PAC learning

Supervised learning framework

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- Generalization error or risk:

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- After that: Linear models.

With probability $\geq 1-\delta$ over samples S, the generalization risk $R(h_S)$ of an ERM rule h_S

Probably

$$\longrightarrow \boxed{R(h_S) < \underbrace{\frac{1}{m} \log\left(\frac{|\mathcal{H}|}{\delta}\right)}_{\text{approximately correct}}}$$

Set $\delta := e^{-m\varepsilon}|\mathcal{H}|$

Proof:

Realizability assumption: With probability 1, there is some $h \in \mathcal{H}$ s.t.

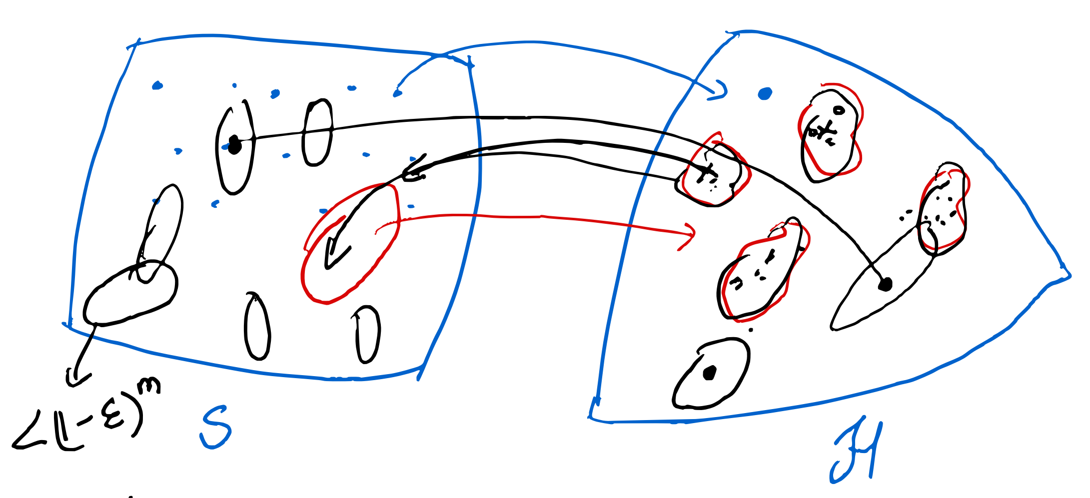
$$h(x) = y$$

$$\boxed{\text{Recall } R(h) = \mathop{\mathbb{E}}_{z \sim D} \ell(z, h)}$$

$$\boxed{h_S \in \underset{h\in\mathcal{H}}{\arg\min}\ \hat{R}_S(h) = \underset{h\in\mathcal{H}}{\arg\min} \frac{1}{m}\sum_{z\in S} \ell(z,h)}$$

For any S, ERM rule h_S is s.t.

$$\hat{R}_S(h_S) = 0$$



$$\mathcal{H}_B \subseteq \mathcal{H}$$

$$\boxed{\mathcal{H}_B := \{h \in \mathcal{H} : R(h) > \varepsilon\}}$$

$$R(h_S) > \varepsilon$$

$$D^m(\{S : h_S \in \mathcal{H}_B\})$$

$$\leq D^m(\{S : (\hat{R}_S(h) = 0) \text{ and } (h \in \mathcal{H}_B)\})$$

Prob review

$$D(A) = \Pr(X \in A) \qquad X \sim D$$

$$= \mathop{\mathbb{E}}_{X\sim D} \mathbb{1}_A(X)$$

$$\mathop{\mathbb{E}}_{X\sim D} f(X) = \sum_{x} f(x) \Pr(X = x) \quad \text{(Discrete)}$$

$$= \int f(x)\, dD(x) \quad \text{(cont)}$$

$$D^m \qquad S = (X_1, \dots, X_m)$$

$$D^m(\{S : (\hat{R}_S(h) = 0) \text{ and } (h \in \mathcal{H}_B)\})$$

$$h(x_i) = y_i \quad \forall\, i \in \{1, 2, \dots, m\}$$

$$D^m(\{S : (\hat{R}_S(h) = 0) \text{ and } (h \in \mathcal{H}_B)\})$$

$$\leq (1-\varepsilon)^m |\mathcal{H}_B| \quad \text{(Union bound)}$$

$$\leq e^{-m\varepsilon} |\mathcal{H}_B|$$

$$\leq e^{-m\varepsilon} |\mathcal{H}| =: \delta$$

Prob review

$$P(A \cup B) \leq P(A) + P(B)$$

$$(1-\varepsilon)^m$$

$$P(A) < \delta$$

$$P(A^c) > 1-\delta$$

$|A|$: size of set A.

$\mathcal{D}^m$: input distribution

$\mathcal{H}$: hypothesis class

"Complexity"

Linear models

$$\mathcal{H} = \{h(\cdot, w, b) : h(x, w, b) = \underline{w \cdot \Phi(x)} + b, w \in \mathbb{R}^d, b \in \mathbb{R}\} \quad (1)$$

$A(x)$ if $A(cx) = cA(x)$

$A(x_1 + x_2) = A(x_1) + A(x_2)$

$\Phi(x) \in \mathbb{R}^d$

$$\begin{bmatrix} w_1 & w_2 & \cdots & w_d & b \end{bmatrix} \begin{bmatrix} \Phi(x)_1 \\ \vdots \\ \Phi(x)_d \\ 1 \end{bmatrix}$$

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- $$\operatorname{argmin}_{w,b} \frac{1}{m} \sum_{i=1}^{m} (w^\top \Phi(x_i) + b - y_i)^2$$

$$[w, b] = \underset{w,b}{\operatorname{argmin}} \frac{1}{m} \sum_{z \in S} \ell(z, h(w, b, \cdot))$$

$$= \underset{w,b}{\operatorname{argmin}} \frac{1}{m} \sum_{\substack{z \in S \\ \downarrow \\ (x,y)}} (w^T \Phi(x) + b - y)^2$$

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- Equivalently, where X is $m \times (d+1)$ matrix with rows $X_i = (\Phi(x_i)^\top, 1)$, $W = [w_1, \cdots, w_d, \cancel{1}\, b]^\top$, $Y = [y_1, \cdots, y_m]^\top$,

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  $$\operatorname{argmin}_W \frac{1}{m} \|X\underline{\underline{W}} - Y\|^2$$
- Features may be defined by kernels

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- $X^T XW = X^T Y$. Can also get this by differentiating before writing in matrix form
- When is $X^T X = \sum_{i=1}^{m} \Phi(x_i)\Phi(x_i)^T$ invertible? When the training features span $\mathbb{R}^d$.

Least squares solutions: the linear algebraic way

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$XW = Y$

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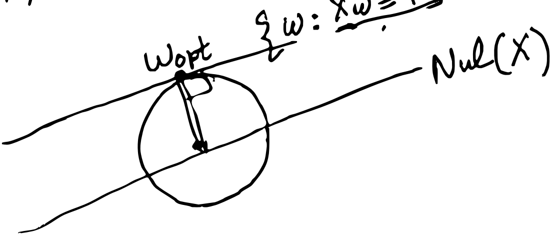
$$\underline{W = X^\top (XX^\top)^{-1} Y}$$

$$\frac{1}{m}\|XW - Y\|^2$$

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$



$$\underset{m\times(d+1)}{X} = \begin{bmatrix} \Phi(x_1) \\ \vdots \\ \Phi(x_m) \end{bmatrix}$$

$$W \in \mathbb{R}^{(d+1)}$$

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- Can solve normal equations above directly, or use iterative methods for linear systems. Cost $\mathcal{O}(d^3)$

Gauss Markov theorem

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- Since $DD^\top$ is positive semi-definite, qed.

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- to derive OLS, also can take derivative and set it to zero. Similarly here.
- Equivalent formulation: $\min_w \sum_{i=1}^m (w^\top \Phi(x_i) - y_i)^2$ subject to $\|w\|^2 \leqslant \Lambda^2$

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- Shrinkage by l^2 regularization.

Generalization of regression

Hoeffding's inequality: $S_n = X_1 + X_2 + \cdots + X_n$

$X_i \perp\!\!\!\perp X_j \quad 0 \le X_i \le L$

$$\mathbb{P}(S_n - \mathbb{E}S_n \geq t) \leq e^{-\frac{2t^2}{nL^2}}$$

Thm: $\sup_{z,h} \ell(z,h) = L$. Let $\mathcal{H}$ be finite.

Then, for every $\delta > 0$, with probability at least $1-\delta$, $\forall\, h \in \mathcal{H}$,

$$R(h) \leq R_S(h) + L\sqrt{\frac{\log|\mathcal{H}| + \log 1/\delta}{2m}}$$