Stefan Bielmeier Homework 3 - Nov 2nd 2021

Problem 1)

Goal: write $P(Y=1|X) = \frac{1}{1+\exp(-b+w^T X)}$ in terms of

- $\pi = P(Y=1)$ (Bernoulli variable outcome - binary)
- μ_{jk} = mean of Gaussian for $k \in \{0,1\}$
- $X_j \sim \mathcal{N}(\mu_{jk}, \sigma_j)$ for $j = 1, \dots, d$ features
- Cond. independence of $X_1, X_2, X_3 \dots$ given $Y = k$

$\Rightarrow$ Bayes: $P(Y=1|X) = \frac{P(X|Y=1)\cdot P(Y=1)}{P(X)}$ where $P(X) = P(X|Y=1)\cdot P(Y=1) + P(X|Y=0)\cdot P(Y=0)$

$$= \frac{P(X|Y=1)\cdot P(Y=1)}{P(X|Y=1)\cdot P(Y=1) + P(X|Y=0)\cdot P(Y=0)}$$

$$= \frac{1}{1 + \frac{P(X|Y=0)\cdot P(Y=0)}{P(X|Y=1)\cdot P(Y=1)}}$$

with conditional independence of features:

$$P(X|Y=0)\cdot P(Y=0) = P(Y=0)\cdot \prod_{j=1}^{d} P(X_j|Y=0)$$

and $P(X|Y=1)\cdot P(Y=1) = P(Y=1)\cdot \prod_{j=1}^{d} P(X_j|Y=1)$ (chain rule)

$$= \frac{1}{1 + \frac{P(Y=0)}{P(Y=1)}\cdot \frac{\prod_{j=1}^{d} P(X_j|Y=0)}{\prod_{j=1}^{d} P(X_j|Y=1)}}$$

$$= \frac{1}{1 + \left(\frac{1-\pi}{\pi}\right)\cdot \frac{\prod_{j=1}^{d} P(X_j|Y=0)}{\prod_{j=1}^{d} P(X_j|Y=1)}}$$

with $P(X_j|Y=k) = \frac{1}{\sqrt{2\pi\sigma_j^2}} \cdot \exp\left(\frac{-(X_j-\mu_{jk})^2}{2\sigma_j^2}\right)$

Substituting, we get

$$\Rightarrow \frac{\prod_{j=1}^{d} P(X_j|Y=0)}{\prod_{j=1}^{d} P(X_j|Y=1)} = \frac{\prod_{j=1}^{d} \frac{1}{\sqrt{2\pi\sigma_j^2}} \cdot \exp\left(\frac{-(X_j-\mu_{j0})^2}{2\sigma_j^2}\right)}{\prod_{j=1}^{d} \frac{1}{\sqrt{2\pi\sigma_j^2}} \cdot \exp\left(\frac{-(X_j-\mu_{j1})^2}{2\sigma_j^2}\right)}$$

$$= \prod_{j=1}^{d} \exp\left(\frac{-(X_j-\mu_{j0})^2}{2\sigma_j^2} - \frac{-(X_j+\mu_{j1})^2}{2\sigma_j^2}\right)$$

$$= \prod_{j=1}^{d} \exp\left(\frac{-X_j^2 + 2\mu_{j0}X_j - \mu_{j0}^2 + X_j^2 - 2\mu_{j1}X_j + \mu_{j1}^2}{2\sigma_j^2}\right)$$

$$= \prod_{j=1}^{d} \exp\left(\frac{\mu_{j0}-\mu_{j1}}{\sigma_j^2} \cdot X_j + \frac{\mu_{j1}^2 - \mu_{j0}^2}{2\sigma_j^2}\right)$$

$\Rightarrow$ back into other equation:

$$P(Y=1|X) = \frac{1}{1 + \frac{1-\pi}{\pi} \cdot \prod_{j=1}^{d} \exp\left(\frac{\mu_{j0}-\mu_{j1}}{\sigma_j^2} \cdot X_j + \frac{\mu_{j1}^2 - \mu_{j0}^2}{2\sigma_j^2}\right)} \quad \left(\text{we count } \frac{1}{1+\exp(\dots)}\right)$$

$$= \frac{1}{1 + \exp\left(\ln\left(\frac{1-\pi}{\pi} \cdot \prod_{j=1}^{d} \exp(\dots)\right)\right)} = \frac{1}{1 + \exp\left(\ln\left(\frac{1-\pi}{\pi}\right) + \ln \prod_{j=1}^{d} \exp(\dots)\right)}$$

$$= \frac{1}{1 + \exp\left(\ln\left(\frac{1-\pi}{\pi}\right) + \sum_{j=1}^{d} \frac{\mu_{j0}-\mu_{j1}}{\sigma_j^2} \cdot X_j + \frac{\mu_{j1}^2 - \mu_{j0}^2}{2\sigma_j^2}\right)}$$

$$= \frac{1}{1+\exp\left(-\underbrace{\left(-\ln\left(\frac{1-\pi}{\pi}\right) - \sum_{j=1}^{d}\frac{\mu_{j1}^2-\mu_{j0}^2}{2\sigma_j^2}\right)}_{b} + \underbrace{\sum_{j=1}^{d}\frac{\mu_{j0}-\mu_{j1}}{\sigma^2}}_{\omega_j}\cdot\underbrace{X_j}_{X_j}\right)}$$

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"Vector"

X_j !

$$\hat{=} \frac{1}{1+\exp\left(-b+\omega^T\cdot X\right)}$$ ✓✓

Problem 2)

a) i) Simple case of X_1 and X_2

$\Rightarrow Var(X_1+X_2) = Var(X_1) + 2Cov(X_1,X_2) + Var(X_2)$

knowing that $Cov(X_1,X_2)=0$ because they're independent variables,

$Var(X_1+X_2) = Var(X_1) + Var(X_2) - \sum_{i=1}^{2} Var(X_i)$

$\Rightarrow Var\left(\underbrace{\frac{\sum_{i=1}^{N} X_i}{n}}_{\text{Average}}\right) = \frac{1}{n^2} Var\left(\sum_{i=1}^{N} X_i\right) = \frac{1}{n^2}\sum_{i=1}^{n} Var(X_i)$ (all X_i's indep.)

with $Var(cX) = c^2 Var(X)$

$= \frac{1}{n^2}\sum_{i=1}^{n}\sigma_i^2$, with all variances the same: $\sigma_i^2 = \sigma^2$

$= \frac{1}{n^2}\cdot n\cdot\sigma^2 = \frac{\sigma^2}{n}$

b) Simple: $P(\text{"data point not chosen in 1 draw"}) = 1-\frac{1}{M}$ (Single random draw from M)

Drawing M times: $P(OOB) = \left(1-\frac{1}{M}\right)^M$

for large M: $\lim_{M\to\infty}\left(1-\frac{1}{M}\right)^M = \frac{1}{e} \approx 0.37$ ✓✓

$$= \frac{1}{1+\exp\left(-\underbrace{\left(-\ln\left(\frac{1-\pi}{\pi}\right) - \sum_{j=1}^{d}\frac{\mu_{j1}^2-\mu_{j0}^2}{2\sigma_j^2}\right)}_{b} + \underbrace{\sum_{j=1}^{d}\frac{\mu_{j0}-\mu_{j1}}{\sigma^2}}_{\omega_j}\cdot X_j\right)}$$

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"Vector" ω_j X_j !

$$\hat{=} \frac{1}{1+\exp\left(-b+\omega^T \cdot X\right)} \quad \checkmark\checkmark$$

Problem 2)

a) i) Simple case of X_1 and X_2

$\Rightarrow Var(X_1+X_2) = Var(X_1) + 2Cov(X_1,X_2) + Var(X_2)$

knowing that $Cov(X_1,X_2)=0$ because they're independent variables, $Var(X_1+X_2) = Var(X_1) + Var(X_2) - \sum_{i=1}^{2} Var(X_i)$

$$\Rightarrow Var\left(\underbrace{\frac{\sum_{i=1}^{N} X_i}{n}}_{\text{Average}}\right) = \frac{1}{n^2} Var\left(\sum_{i=1}^{N} X_i\right) = \frac{1}{n^2}\sum_{i=1}^{n} Var(X_i) \quad (\text{all } X_i\text{s indep})$$

with $Var(cX) = c^2 Var(X)$

$$= \frac{1}{n^2}\sum_{i=1}^{n}\sigma_i^2 \quad \text{, with all variances the same: } \sigma_i^2 = \sigma^2$$

$$= \frac{1}{n^2}\cdot n\cdot\sigma^2 = \frac{\sigma^2}{n}$$

ii) Simple: $P(\text{"data point not chosen in 1 draw"}) = 1-\frac{1}{M}$ (Single random draw from M)

Drawing M times: $P(OOB) = \left(1-\frac{1}{M}\right)^M$

for large M: $\lim_{M\to\infty}\left(1-\frac{1}{M}\right)^M = \frac{1}{e} \approx 0.37$ $\checkmark\checkmark$

a iii) The OOB error works the following way:

1) generate B samples of length n of dataset with length n.
2) Train a model on each sample B_1, B_2, etc.
3) Deliberately make models do a prediction on an observation that they didn't include in training sample.
4) Average that prediction, and compare to real value ≙ OOB error for single observation
5) Do for all observations
   ↳ OOB error = $\frac{\text{Falsely pred. observations (OOB)}}{\text{all observations (OOB)}}$

→ The OOB error decreases for a given model with the more trees it has ⇒ is better able to classify observations it "didn't know".

→ At some point, increasing the # of trees will become computionally more expensive, while the OOB error only decreases slightly / marginally less

→ Choose the # of trees when OOB isn't decreasing significantly anymore.

2a iv)

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- Var for correlated random vars $X_1, X_2, \dots, X_n$

$$\Rightarrow \operatorname{Var}\left(\frac{\sum_{i=1}^{n} X_i}{n}\right) = \frac{1}{n^2} \cdot \operatorname{Var}\left(\sum_{i=1}^{n} X_i\right)$$

$$= \frac{1}{n^2}\left(\sum_{i=1}^{n} \operatorname{Var}(X_i) + \sum_{i=1}^{n}\sum_{i \neq j} \operatorname{Cov}(X_i, X_j)\right)$$

upper bound: $\leq \frac{1}{n^2} \cdot \left(n \cdot \sigma_i^2 + n \cdot (n-1) \cdot \delta^2\right)$ (with $\operatorname{Cov}(X_i, X_j) \leq \delta^2$)

$\leq \frac{1}{n^2} \cdot \left(n \cdot \sigma^2 + (n^2 - n)\delta^2\right)$ with $\sigma_i^2 = \sigma^2$

$\leq \frac{1}{n^2} \cdot \left(n\sigma^2 + (n^2 - n)\delta^2\right)$

$\leq \frac{\sigma^2}{n} + \frac{n^2\delta^2 - n\delta^2}{n^2} = \frac{\sigma^2}{n} + \delta^2 - \frac{\delta^2}{n}$

$\leq \underline{\frac{1}{n} \cdot \sigma^2 + \left(1 - \frac{1}{n}\right) \cdot \delta^2}$

v) with $N \to \infty$:

$$\lim_{n \to \infty} \underbrace{\frac{1}{n}}_{\to 0} \sigma^2 + \underbrace{\left(1 - \frac{1}{n}\right)}_{\to 0} \cdot \delta^2 = 0 + (1 - 0)\delta^2 = \delta^2$$

from part i: $\lim_{n \to \infty} \frac{\sigma^2}{n} = 0$

$\Rightarrow$ Bagging is limited by the covariance of the dataset's features or random variables (which we see in the trees' covariance).

$\Rightarrow$ Bagging is limited by the degree of correlation between the trees.

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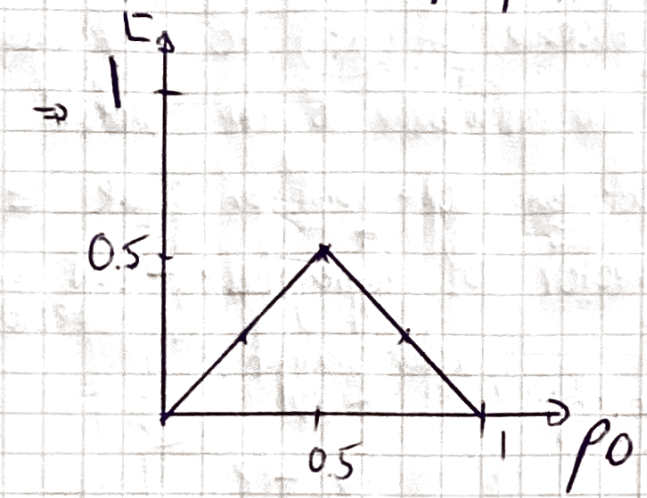
2b) $E = 1 - \max_k p_k$ with $k \in \{0,1\}$

$= 1 - \max(p_1, p_0)$ with $p_0 = 1 - p_1$

(classification error rate)



! we use p_0 as first class ! (doesn't matter for plots)

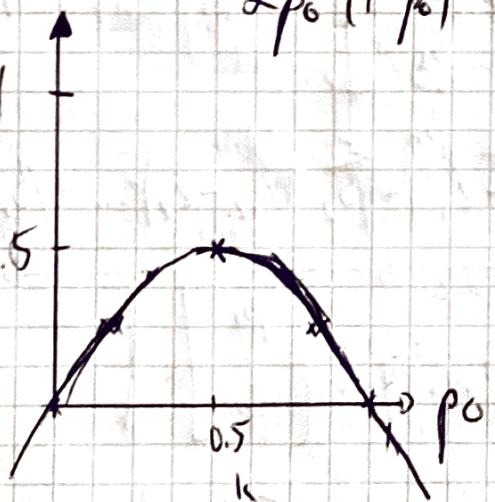
Gini-Index:

$\sum_{k=1} p_k(1-p_k)$, starting at $k=0$ with $k \in \{0,1\}$

$\Rightarrow \sum_{k=0} p_k(1-p_k) = p_0(1-p_0) + p_1(1-p_1) = p_0 \cdot p_1 + p_1 p_0 = 2p_1 p_0$

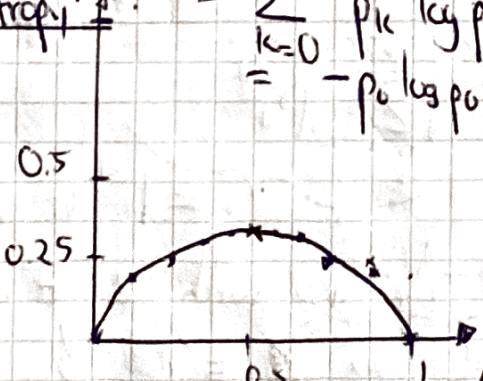
$= 2p_0 \cdot (1-p_0) = -2p^2 + 2p_0$

$\Rightarrow$



Entropy: $-\sum_{k=0}^{k} p_k \log p_k = -(p_0 \log p_0 + p_1 \log p_1)$

$= -p_0 \log p_0 - (1-p_0)\log(1-p_0)$



Problem 3a)

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we want to calculate the distance of x_i to hyperplane (perpendicular distance). That is equivalent to the scalar projection of b (vector between same point on plane z and x_i) on n (normal vector of hyperplane - unit normal vector)

$$d = |\text{comp}_n b| = \frac{|b \circ n|}{|n|} \quad \text{with: } \circ \text{ scalar product.}$$

$$x_i = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \dots \\ x_{in} \end{bmatrix} \quad z = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \\ \vdots \\ z_n \end{bmatrix} \Rightarrow b = \begin{bmatrix} x_{i1} - z_1 \\ x_{i2} - z_2 \\ \dots \\ x_{in} - z_n \end{bmatrix}$$

and $n = \frac{\langle w \rangle}{|w|}$ with $\langle w \rangle$ is $\beta_1, \beta_2 \dots, \beta_n$ (weights of hyperplane)

$$= \frac{1}{\sqrt{\beta_1^2 + \beta_2^2 + \dots + \beta_n^2}} \cdot \begin{bmatrix} \beta_1 \\ \beta_2 \\ \dots \\ \beta_n \end{bmatrix}$$

$$\Rightarrow d = \frac{\left| \frac{1}{\sqrt{\beta_1^2 + \beta_2^2 + \dots + \beta_n^2}} \cdot \left(\beta_1 \cdot (x_{i1} - z_1) + \beta_2 \cdot (x_{i2} - z_2) + \dots + \beta_n \cdot (x_{in} - z_n) \right) \right|}{\sqrt{\frac{1}{\sqrt{\beta_1^2 + \beta_2^2 + \dots + \beta_n^2}} \cdot \begin{bmatrix} \beta_1 \\ \dots \\ \beta_n \end{bmatrix}}}$$

with $\left| \begin{bmatrix} \beta_1 \\ \dots \\ \beta_n \end{bmatrix} \right| = \sqrt{\sum_{j=1}^{p} \beta_j^2}$

$$:= \frac{|\beta_1 \cdot x_{i1} + \beta_2 \cdot x_{i2} + \dots \beta_n \cdot x_{in} - \beta_1 \cdot z_1 - \beta_2 \cdot z_2 - \dots - \beta_n \cdot z_n|}{\sqrt{\sum_{j=1}^{p} \beta_j^2}}$$

$\sqrt{\sum_{j=1}^{p} \beta_j^2} = 1$ (constraint)

and with $(-\beta_1 \cdot z_1 - \beta_2 \cdot z_2 - \dots - \beta_n \cdot z_n)$ with $z \in$ hyperplane

$\Rightarrow \beta_1 \cdot z_1 + \beta_2 \cdot z_2 + \dots + \beta_n \cdot z_n + \beta_0 \overset{!}{=} 0 \Rightarrow = \beta_0$

$$\Rightarrow d = |\beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_n x_{in} + \beta_c|$$
$$= |\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}|$$

now: max margin classifier: Classify based on sign of $f(x_i)$ with $f(x_i) = \beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}$

$\Leftrightarrow$ $\text{sign}(y_i) = \text{sign}(\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij})$

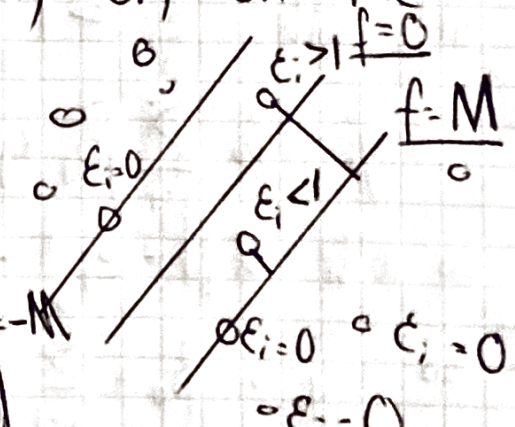
$\Rightarrow d = y_i \cdot (\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}) = |\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}|$

$(-1 \cdot -1 = 1,\ 1 \cdot 1 = 1)$ ✓

Problem 3b)

(i) given point x_i, with $\varepsilon_i = 0$

$d \geq M \cdot (1 - \varepsilon_i) \Rightarrow d \geq M$ x_i is on the correct side of margin ✓ (on either side) or, on the margin support vector!, at least $\geq M$ away from hyperplane



as x_i has a distance d to hyperplane, that is $\geq M$, we can safely assume that it's classified correctly $\Rightarrow$ On correct side of hyperplane. ✓

We know that the optimization problem will fulfill this constraint $\text{sign}(y_i) \cdot \text{sign}(d_{raw}) \geq M$ $\Rightarrow$ needs to be equal sign $\Rightarrow$ correct class!

3b ii)

$0 < \varepsilon_i < 1$ for point x_i

⇒ is it on the correct side of the hyperplane?

↳ $y_i \left(\beta_0 + \sum_{j=1}^{p} \beta_j \cdot x_{ij}\right) \geq M \cdot (1 - \varepsilon_i)$ with $0 < \varepsilon_i < 1$

⇒ $0 < y_i \left(\beta_0 + \sum_{j=1}^{p} \beta_j \cdot x_{ij}\right) < M$

⇒ point x_i is classified correctly, (signs of y_i must match $\beta_0 + \sum_{j=1}^{p} \beta_j \cdot x_{ij}$ to satisfy inequality above)
(not on the hyperplane as $d > 0$)
however, a loss incurred because $\varepsilon_i > 0$.

The point x_i is not on the correct side of the margin, but between the hyperplane and the margin support vector,

with $0 < d(x_i) < M$

iii) with $\varepsilon_i > 1$ for x_i (one point)

$y_i \cdot \left(\beta_0 + \sum_{j=1}^{p} \beta_j \cdot x_{ij}\right) \geq M \cdot (1 - \varepsilon_i)$

⇒ with $M \cdot (1 - \varepsilon_i) < 0$ for $\varepsilon_i > 1$

⇒ $y_i \cdot \left(\beta_0 + \sum_{j=1}^{p} \beta_j \cdot x_{ij}\right) < 0$ (has a negative sign)

⇒ Misclassified, as $\text{sign}(y_i) \neq \text{sign}\left(\beta_0 + \sum_{j=1}^{p} \beta_j \cdot x_{ij}\right)$

⇒ Not on correct side of hyperplane,

⇒ Not on correct side of the margin!

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3c)

Show that $f(x^*) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x^*, x_i \rangle$

is equal to $f(x^*) = \beta_0 + \beta_1 x_1^* + \beta_2 x_2^* + \dots + \beta_p \cdot x_p^*$,

with: $\mathbb{R}^p$, and x_i^{th} notes the i^{th} training observation.

⊕ ⇒ Find values for β_j, $j \in \{1, \dots, p\}$ in terms of α_i & x_i for $i \in \{1, \dots, n\}$

$$\Rightarrow f(x^*) = \beta_0 + \sum_{i=1}^{n} \alpha_i \cdot \langle x^*, x_i \rangle \quad \text{with } \langle x^*, x_i \rangle = (x_1^* \cdot x_{i1} + x_2^* \cdot x_{i2} + \dots + x_p^* \cdot x_{ip}) \text{ (Scalar product)}$$

$$= \beta_0 + \sum_{i=1}^{n} \alpha_i \left(x_1^* \cdot x_{i1} + x_2^* \cdot x_{i2} + \dots + x_p^* \cdot x_{ip} \right)$$

$$= \beta_0 + \sum_{i=1}^{n} \alpha_i \cdot \sum_{j=1}^{p} x_j^* \cdot x_{ij} \quad \text{(we want } \textstyle\sum_{j=1}^{p} \text{ outside)}$$

$$= \beta_0 + \sum_{i=1}^{n} \sum_{j=1}^{p} \alpha_i x_j^* \cdot x_{ij} = \beta_0 + \sum_{j=1}^{p} x_j^* \sum_{i=1}^{n} \alpha_i \cdot x_{ij}$$

$$= \beta_0 + x_1^* \cdot \sum_{i=1}^{n} \alpha_i \cdot x_{i1} + x_2^* \cdot \sum_{i=1}^{n} \alpha_i x_{i2} + \dots + x_p^* \cdot \sum_{i=1}^{n} \alpha_i x_{ip}$$

$$\Rightarrow \text{with } \underline{\beta_j = \sum_{i=1}^{n} \alpha_i \cdot x_{ij}} \text{ for all } j \in \{1, \dots, p\}$$

$$\hat{=} \beta_0 + x_1^* \cdot \beta_1 + \dots + x_p^* \cdot \beta_p \quad \checkmark\checkmark$$