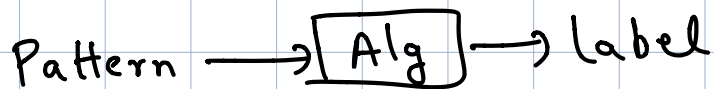


Classification task



Notation:

① \mathcal{X} : Feature space = Set of all feature vectors
For eg. $\mathcal{X} = \mathbb{R}^d$

② Classifier $h: \mathcal{X} \rightarrow \{1, \dots, M\}$

Simple case: $M=2$, $\{0, 1\}$ or $\{-1, +1\}$

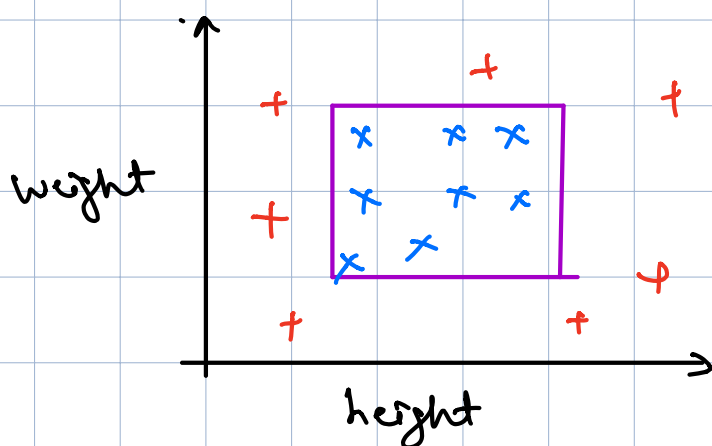
How to design classifiers & how to judge their performance?

Input: $\{(x_i, y_i), i=1 \dots n\}$ Training dataset
 \uparrow feature vector \nwarrow class label

Using training data, learn an appropriate classifier h

Test! Test & validate the h on "new" data

Example: Medium-build



Regression task:

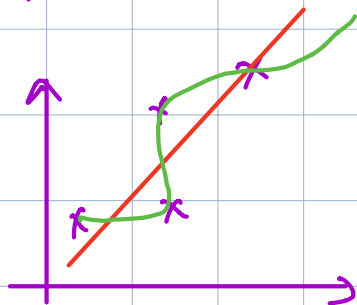
Training data: $\{(x_i, y_i), i=1 \dots n\}$
 $x_i \in \mathbb{R}^d, y_i \in \mathbb{R}$

Need is to learn a function $h: \mathcal{X} \rightarrow \mathbb{R}$

Examples: prediction of stock prices, etc

Curve-fitting: $\{(x_1, y_1), \dots, (x_n, y_n)\}$

Find a function f s.t. $y = f(x)$



Generalization:- Obtain a classifier/regression function

using a training dataset s.t. the error on "unseen" (test) data is low.

Assumption: There is a distribution underlying the data.

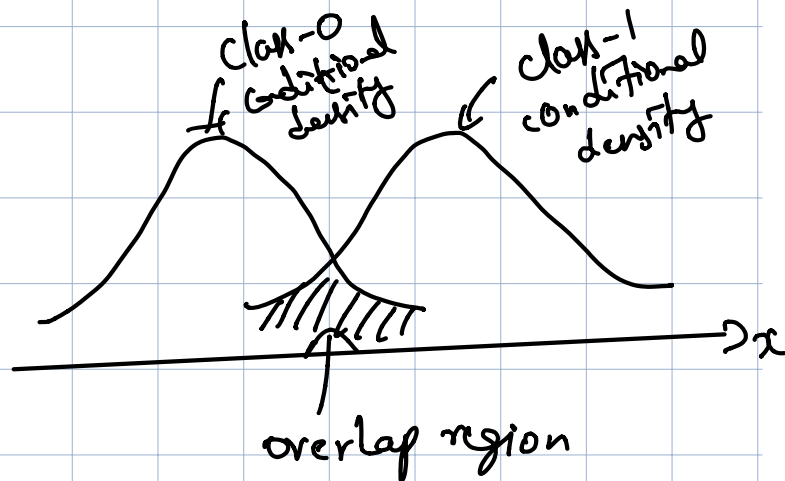
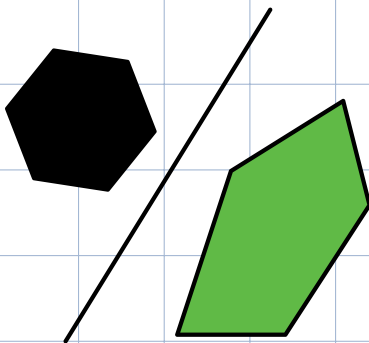
Formally,

f_i : conditional density of features from class - i

Let $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ represent a feature vector

$f_i(x)$: joint density of (x_1, \dots, x_d) given that x is in class - i

Note: A feature vector x can belong to different classes with different probabilities



X : feature space

$Y = \{0, 1\}$ class-labels

$H =$ set of classifiers $= \{h \mid h: X \rightarrow Y\}$

Performance metric: $F(h) = P(h(x) \neq y(x))$

\downarrow
Probability of mis-classification

\uparrow label assigned by classifier h \uparrow true class label

Goal: $h^* = \operatorname{argmin}_{h \in H} F(h)$

Bayes classifier

Let $P_i = P(Y(X) = i) \leftarrow$ prior probabilities

$q_i(x) = P(Y(X) = i \mid X=x)$

Bayes classifier $h_B(x) = \begin{cases} 0 & \text{if } \frac{q_0(x)}{q_1(x)} > 1 \\ 1 & \text{else} \end{cases}$

P 10

From Bayes Theorem,

posterior \propto prior \times likelihood

$$q_i(x) = \frac{p_i f_i(x)}{p_0 f_0(x) + p_1 f_1(x)}$$

\hookrightarrow Normalizing constant

Bayes classifier:

Classify x as "belonging to class 0"

$$\text{if } q_0(x) > q_1(x)$$

$$\Leftrightarrow p_0 f_0(x) > p_1 f_1(x)$$

Optimality of Bayes classifier:

Fix a classifier h

Define $R_i(h) = \{x \in X \mid h(x) = i\}$, $i = 0, 1$

$$F(h) = P(h(x) \neq y(x))$$

$$= P(x \in R_1(h), x \in \text{class-0})$$

$$+ P(X \in R_0(h), X \in \text{class-1})$$

$$= P_0 P(X \in R_1(h) | X \in \text{class-0})$$

$$+ P_1 P(X \in R_0(h) | X \in \text{class-1})$$

$$= P_0 \int_{R_1(h)} f_0(x) dx + P_1 \int_{R_0(h)} f_1(x) dx$$

For the Bayes classifier h_B :

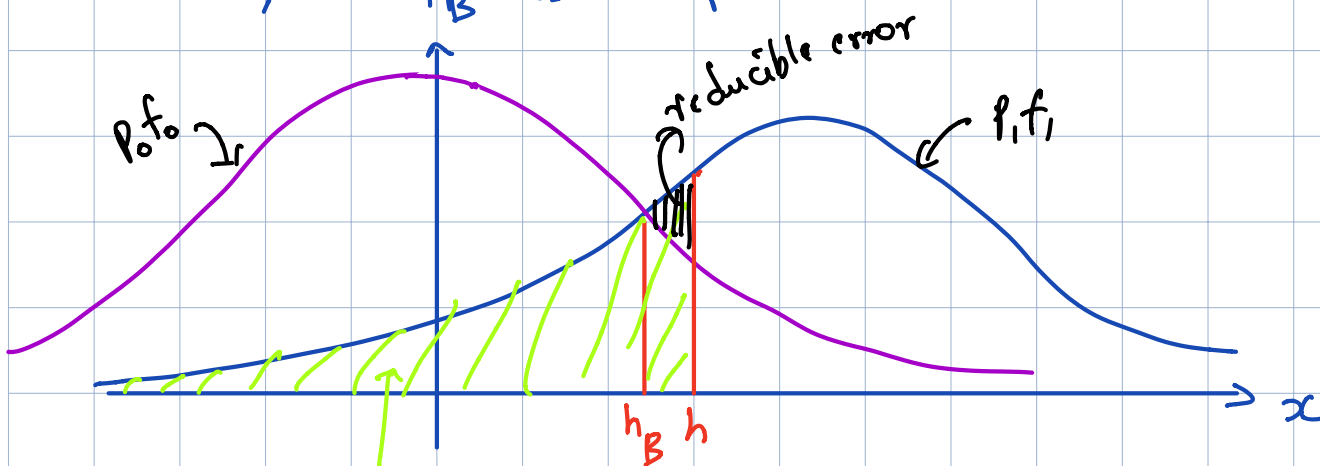
$$R_0(h_B) = \{x \mid P_0 f_0(x) \geq P_1 f_1(x)\}$$

$$R_1(h_B) = \{x \mid P_1 f_1(x) > P_0 f_0(x)\}$$

$$\text{So, } F(h_B) = \int_{R_1(h)} P_0 f_0(x) dx + \int_{R_0(h)} P_1 f_1(x) dx$$

$$= \int \min(P_0 f_0(x), P_1 f_1(x)) dx$$

So, h_B is optimal.



$$\int_{\mathcal{X}} P_i f_i(x) dx$$

Generalizing Bayes classifier to handle loss functions:-

Loss function $L: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}^+$

$L(h(x), y(x))$ is the loss suffered by h on pattern x .

Performance metric $F(h) = E[L(h(x), y(x))]$

Special case:- $(0-1)$ loss function $\rightarrow L(a, b) = \begin{cases} 0 & \text{if } a = b \\ 1 & \text{if } a \neq b \end{cases}$

Then, $F(h) = P(h(x) \neq y(x))$ for above L .

In general, $L(0, 1) \neq L(1, 0)$ [$L(0, 0) = L(1, 1) = 0$]

h_B for optimizing (*) is

$$h_B(x) = \begin{cases} 0 & \text{if } \frac{q_0(x)}{q_1(x)} > \frac{L(0, 1)}{L(1, 0)} \\ 1 & \text{else} \end{cases}$$

Note: If $L(1, 0) = L(0, 1)$, we recover the Bayes classifier for 0-1 loss function

Extending Bayes classifier to multi-class classification problems:-

Let $\{0, 1, \dots, M-1\}$ be the M -class labels.

$L(i, j) \rightarrow$ loss function
Classifier predicts i true class label j

$$R(h) = E(L(h(x), y(x))) \leftarrow (x, x)$$

Goal: minimize $R(h)$

Deriving the Bayes classifier:

$$\begin{aligned} \text{Let } R(i|x) &= E(L(h(x), y(x)) | h(x)=i, x) \\ &= E(L(i, y(x)) | \text{---}) \\ &= \sum_{j=0}^{M-1} L(i, j) P(y(x)=j|x) \\ &= \sum_{j=0}^{M-1} L(i, j) q_j(x) \end{aligned}$$

$$\begin{aligned} R(h) &= E(E(L(h(x), y(x)) | x)) \\ &= \int R(h(x)|x) f(x) dx \end{aligned}$$

need to minimize this $\forall x \in \mathcal{X}$.

Bayes Classifier:

$$h_B(x) = i \quad \text{if} \quad \sum_{j=0}^{M-1} L(i,j) q_j(x) \leq \sum_{\substack{j=0 \\ j \neq k}}^{M-1} L(k,j) q_j(x),$$

Claim: h_B is optimal for (***)

Special Case for $M=2$:

$$h_B(x) = 0 \quad \text{if}$$

$$\begin{aligned} & L(0,0) q_0(x) + L(0,1) q_1(x) \\ & \leq L(1,0) q_0(x) + L(1,1) q_1(x) \end{aligned} \quad \text{--- (***)}$$

If $L(0,0) = L(1,1) = 0$, then (***) is equivalent to

$$\frac{q_0(x)}{q_1(x)} \geq \frac{L(0,1)}{L(1,0)}$$

H.W.: For 0-1 loss function, with a M -class classification problem, derive h_B .

Special Case: $X \in \mathbb{R}$

$$f_i \sim N(\mu_i, \sigma_i^2), \quad i=0,1$$

$$f_i(x) = \frac{1}{\sqrt{2\pi} \sigma_i} \exp\left(-\frac{(x-\mu_i)^2}{2\sigma_i^2}\right), \quad i=0,1$$

$$h_B(x) = 0 \quad \text{if}$$

$$P_0 f_0(x) L(1,0) > P_1 f_1(x) L(0,1)$$

$$\log(P_0 L(1,0)) + \log(f_0(x)) > \log(P_1 L(0,1)) + \log(f_1(x))$$

\leftarrow ~~(****)~~

$$\log(P_0 L(1,0)) - \log(\sigma_0) - \frac{1}{2} \log(2\pi) - \frac{(x-\mu_0)^2}{2\sigma_0^2}$$

$$> \log(P_1 L(0,1)) - \log(\sigma_1) - \frac{1}{2} \log(2\pi) - \frac{(x-\mu_1)^2}{2\sigma_1^2}$$

$$\frac{1}{2} x^2 \left(\frac{1}{\sigma_1^2} - \frac{1}{\sigma_0^2} \right) + x \left(\frac{\mu_0}{\sigma_0^2} - \frac{\mu_1}{\sigma_1^2} \right)$$

$$+ \frac{1}{2} \left(\frac{\mu_1^2}{\sigma_1^2} - \frac{\mu_0^2}{\sigma_0^2} \right) + \log\left(\frac{\sigma_1}{\sigma_0}\right) + \log\left(\frac{P_0 L(1,0)}{P_1 L(0,1)}\right)$$

$$> 0$$

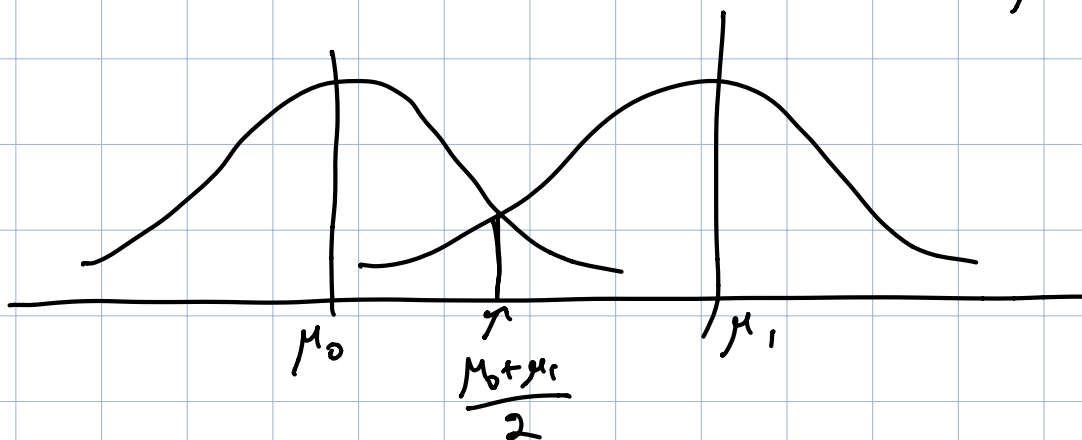
Special Case:

① $\sigma_0 = \sigma_1 = \sigma$, $P_0 = P_1$, $L(1,0) = L(0,1)$ ← equi-probable classes

Then, $h_B(x) = 0$ if

$$\frac{x}{\sigma^2} (\mu_0 - \mu_1) - \frac{1}{2\sigma^2} (\mu_0^2 - \mu_1^2) > 0$$

i.e., $x > \frac{\mu_0 + \mu_1}{2}$ (assuming $\mu_0 > \mu_1$)

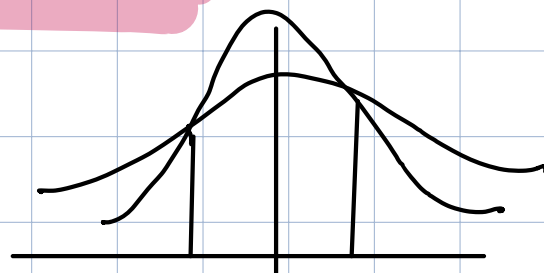


② $\mu_0 = \mu_1 = 0$, $P_0 = P_1$, $L(1,0) = L(0,1)$
 $h_B(x) = 0$ if

$$\frac{x^2}{2} \left(\frac{1}{\sigma_1^2} - \frac{1}{\sigma_0^2} \right) - \log \left(\frac{\sigma_0}{\sigma_1} \right) > 0$$

$\sigma_0 > \sigma_1 \Rightarrow$

$$\frac{x^2}{2} > \frac{\sigma_1^2 \sigma_0^2 \log(\sigma_0/\sigma_1)}{(\sigma_0^2 - \sigma_1^2)}$$



③ Generalization to multivariate class-conditional densities:

$$f_i(x) = \frac{1}{\sqrt{(2\pi)^d |\Sigma_i|}} \exp\left(-\frac{1}{2}(x-\mu_i)^T \Sigma_i^{-1} (x-\mu_i)\right), \quad i=0,1$$

$h_B(x) = 0$ if check!

$$\frac{1}{2} x^T (\Sigma_1^{-1} - \Sigma_0^{-1}) x + x^T (\Sigma_0^{-1} \mu_0 - \Sigma_1^{-1} \mu_1) + \frac{1}{2} (\mu_1^T \Sigma_1^{-1} \mu_1 - \mu_0^T \Sigma_0^{-1} \mu_0)$$

$$+ \log\left(\frac{p_0 L(1,0)}{p_1 L(0,1)}\right) + \frac{1}{2} \log\left(\frac{|\Sigma_1|}{|\Sigma_0|}\right) > 0$$

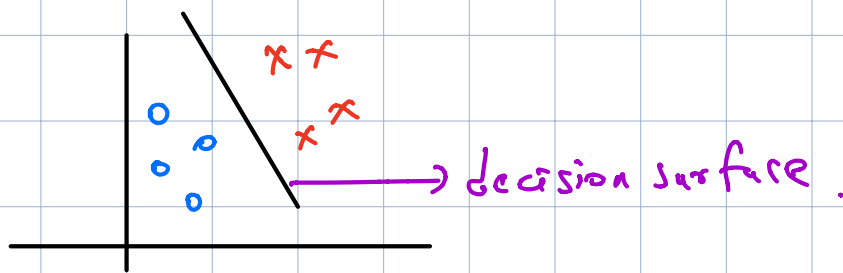
H.W: Work out the special case as in the univariate setting.

DISCRIMINANT FUNCTIONS:

$$h(x) = \begin{cases} 0 & \text{if } g(x) > 0 \\ 1 & \text{else} \end{cases}$$

Example: 0-1 loss function. Bayes classifier is based on the discriminant function $g(x) = q_0(x) - q_1(x)$

$g(x)=0$ is the decision surface.



Maximum likelihood estimation

- ① To implement Bayes classifier, we need class conditional densities & prior probabilities
- ② Suppose we are given i.i.d. samples from a class conditional distribution

$$\{x_1, \dots, x_n\}$$

- ③ We adopt a "parametric" approach to estimation

$\mathcal{D} = \{x_1, \dots, x_n\}$ iid from the distribution of r.v. X parameterized by θ .

Aim: Use \mathcal{D} to estimate θ

Example:

$$f(x|\theta) \sim N(\theta_1, \theta_2)$$

(θ_1, θ_2) unknown

$$f(x|\theta) = \frac{1}{\sqrt{2\pi} \theta_2} \exp\left(-\frac{(x-\theta_1)^2}{2\theta_2^2}\right)$$

$\hat{\theta}_n \leftarrow$ estimate of θ .

Example:- Suppose X is drawn uniformly at random from the set $\{1, \dots, n\}$

Suppose "n" is unknown

Suppose we observe a sample "k".

Want an estimator of n given $X=k$ is observed.

Max-likelihood (ML) idea:

The pmf of X $P_X(k) = \frac{1}{n} \mathbb{I}\{1 \leq k \leq n\}$

Think of $P_X(k)$ as a function of n .

∴ find the maximizer of this function



$P_x(k)$ is 0 for $n \leq k-1$, jumps to $\frac{1}{k}$ at $n=k$ & decreases beyond k . So, it is maximized at $n=k$.

$$\hat{n}_{MC}(k) = k.$$

Suppose we are given $\{x_1, \dots, x_n\}$ iid $\sim f(\cdot | \theta)$

S.g. $x_i \sim N(\theta, 1)$ ← one-parameter distribution, $i=1, \dots, n$
 \uparrow
 unknown

$\hat{\theta}_n$ ← estimate of θ

Sample mean → $\hat{\theta}_n = \frac{1}{n} \sum_{i=1}^n x_i$, $\hat{\theta}_2 = \frac{x_1 + x_2}{2}$, $\hat{\theta}_1 = x_1$

Why choose $\hat{\theta}_n$ over $\hat{\theta}_2$ & $\hat{\theta}_1$?

Use a "mean-square error" objective

$$MSE(\hat{\theta}) = E[(\hat{\theta} - \theta)^2]$$

$$= E\left[\left(\hat{\theta} - E[\hat{\theta}]\right) + \left(E[\hat{\theta}] - \theta\right)\right]^2$$

$$= E\left[(\hat{\theta} - E\hat{\theta})^2\right] + (E(\hat{\theta}) - \theta)^2 + 2 \underbrace{E\left[(\hat{\theta} - E\hat{\theta})(E\hat{\theta} - \theta)\right]}_{=(E\hat{\theta} - \theta)E(\hat{\theta} - E\hat{\theta}) = 0}$$

$$= E \left[\underbrace{(\hat{\theta} - E\hat{\theta})^2}_{\text{variance}} \right] + \underbrace{(E\hat{\theta} - \theta)^2}_{\text{bias}^2}$$

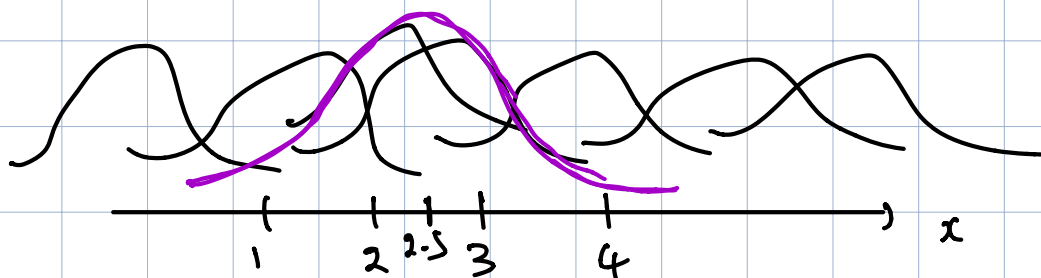
Estimator $\hat{\theta}$ unbiased if $E\hat{\theta} = \theta$

$$\text{Var}(\hat{\theta}_n) = \frac{1}{n}, \quad \text{Var}(\hat{\theta}_2) = \frac{1}{2}, \quad \text{Var}(\hat{\theta}_1) = 1$$

Max-likelihood estimation:

$$\mathcal{D} = \{x_1, \dots, x_n\}$$

e.g. $x_i \sim \mathcal{N}(\theta, 1)$



Likelihood function $L(\theta) = \prod_{j=1}^n f(x_j | \theta)$

ML estimate: $\theta^* \in \arg \max_{\theta} \{L(\theta) = L(x_1, \dots, x_n, \theta)\}$

$$L(\theta^*) \geq L(\theta) \quad \forall \theta$$

Log-likelihood $l(\theta) = \text{Log} L(\theta) = \sum_{j=1}^n \log f(x_j | \theta)$

Example: Univariate normal

$$x_i \sim N(\theta_1, \theta_2^2), i=1, \dots, n$$

$$l(\theta) = \log L(\theta) = \sum_{j=1}^n \left(-\log \theta_2 - \frac{1}{2} \log 2\pi - \frac{(x_j - \theta_1)^2}{2\theta_2^2} \right)$$

$$l(\theta) = -n \log \theta_2 - \frac{n}{2} \log 2\pi - \sum_{j=1}^n \frac{(x_j - \theta_1)^2}{2\theta_2^2}$$

To find ML estimates $\hat{\theta}_1, \hat{\theta}_2$ of θ_1 & θ_2 , do

$$(i) \quad \frac{\partial l}{\partial \theta_1} = 0$$

$$\& \quad (ii) \quad \frac{\partial l}{\partial \theta_2} = 0$$

$$\hat{\theta}_1 = \frac{1}{n} \sum_{j=1}^n x_j$$

$$\hat{\theta}_2^2 = \frac{1}{n} \sum_{j=1}^n (x_j - \hat{\theta}_1)^2$$

not unbiased ↓

h.w.: ① Assume $\text{Exp}(\lambda)$ likelihood & find the ML estimate

② Generalize to multivariate case

$$x_i \sim N(\mu, \Sigma), i=1, \dots, n, x_i \in \mathbb{R}^d$$

Calculate ML estimates for μ, Σ .

$$\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n x_i; \quad \hat{\Sigma}_n = \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\mu}_n)(x_i - \hat{\mu}_n)^T$$

$$\left(\text{recall } \Sigma = E(x-\mu)(x-\mu)^T \right)$$

Example:- Suppose a coin with bias θ is tossed n times & k heads occur.

$$P_{\hat{\theta}}(X=k) = \binom{n}{k} (\hat{\theta})^k (1-\hat{\theta})^{n-k} = L(\hat{\theta})$$

$$\hat{\theta}_{MC} = \arg \max_{\hat{\theta}} (\hat{\theta})^k (1-\hat{\theta})^{n-k}, \quad n, k \text{ known}$$

Let $1 \leq k \leq n-1$

$$\frac{d}{d\hat{\theta}} (\hat{\theta}^k (1-\hat{\theta})^{n-k}) = \frac{k \hat{\theta}^{k-1} (1-\hat{\theta})^{n-k}}{\hat{\theta}} - \frac{(n-k) \hat{\theta}^k (1-\hat{\theta})^{n-k-1}}{(1-\hat{\theta})}$$

$$= \left(\frac{k}{\hat{\theta}} - \frac{(n-k)}{(1-\hat{\theta})} \right) \hat{\theta}^{k-1} (1-\hat{\theta})^{n-k}$$

$$= (k - n\hat{\theta}) \hat{\theta}^{k-1} (1-\hat{\theta})^{n-k-1} \quad \text{--- (x)}$$

If $\hat{\theta} \leq \frac{k}{n}$, then $(x) \geq 0$

if $\hat{\theta} > \frac{k}{n}$, then $(x) < 0$

So, $\hat{\theta}_{MC} = \frac{k}{n}$

For $k=0$, $L(\hat{\theta}) = (1-\hat{\theta})^n$ & $\hat{\theta}_{MC} = 0$

For $k=n$, $L(\hat{\theta}) = \hat{\theta}^n$ & $\hat{\theta}_{MC} = 1$

H.W. (i) Work out ML estimate for (i) Poisson (λ) likelihood. & (ii) Geometric (θ) likelihood

Bayesian estimation

Frequentists	Bayesian
Probability = long run frequency	Probability = degree of belief (subjective)
Goal = algorithms with long-run freq. guarantees	Goal: State & analyze beliefs

Bayesian approach:-

Parameter θ is given a prior density $\pi(\theta)$

Observe data $\{x_1, \dots, x_n\}$ sampled from $f(x|\theta)$

Compute posterior density (use Bayes rule)

$$f(\theta | x_1, \dots, x_n) \propto L(\theta) \pi(\theta)$$

Example:

$$D_n = \{x_1, \dots, x_n\}$$

$$x_i \sim \text{Ber}(\theta)$$

Uniform prior $\pi(\theta) = 1$

Posterior probability \leftarrow prior \leftarrow likelihood

$$f(\theta | \mathcal{D}_n) \propto \pi(\theta) \mathcal{L}_n(\theta)$$

$$\propto 1 \times \prod_{i=1}^n f(x_i | \theta)$$

$$\propto \prod_{i=1}^n \theta^{x_i} (1-\theta)^{1-x_i}$$

$$\propto \theta^{S_n} (1-\theta)^{n-S_n}$$

$$\propto \theta^{(S_n+1)-1} (1-\theta)^{(n-S_n+1)-1}$$

Denote $S_n = \sum_{i=1}^n x_i$

Beta density: $\pi_{\alpha, \beta}(\theta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1} (1-\theta)^{\beta-1}$

so, $f(\theta | \mathcal{D}_n) \sim \text{Beta}(S_n+1, n-S_n+1)$

Posterior - mean = $\frac{S_n+1}{n+2}$

n.w. Redo the calculation above for $\pi(\theta) \sim \text{Beta}(\alpha, \beta)$

Bayes estimation

Working procedure:

- ① Choose a prior density $\pi(\theta)$
- ② Observe data $\mathcal{D}_n = \{x_1, \dots, x_n\}$ sampled i.i.d.
from $f(x|\theta) \leftarrow$ likelihood
- ③ Update beliefs:
Calculate posterior density

$$f(\theta | \underbrace{x_1, \dots, x_n}_{\mathcal{D}_n}) \stackrel{\text{Bayes rule}}{=} \frac{f(x_1, \dots, x_n | \theta) \pi(\theta)}{f(x_1, \dots, x_n)}$$
$$= \frac{L_n(\theta) \pi(\theta)}{\underbrace{\hspace{10em}}_{\text{Normalization constant} \rightarrow C_n}}$$

$$f(\theta | x_1, \dots, x_n) \propto L_n(\theta) \times \pi(\theta)$$

posterior likelihood prior

Point estimates

- ① Posterior mean $\bar{\theta}_n = \int \theta f(\theta | \mathcal{D}_n) d\theta$
- ② Maximum a posteriori probability (MAP)
= mode of the posterior

Example:

$$\mathcal{D}_n = \{x_1, \dots, x_n\}$$

$$x_i \sim \text{Ber}(\theta)$$

Beta prior i.e., $\pi(\theta) \sim \text{Beta}(\alpha, \beta)$

Then,

$$f(\theta | \mathcal{D}_n) \propto \theta^{\alpha-1} (1-\theta)^{\beta-1} \theta^{S_n} (1-\theta)^{n-S_n}$$
$$\propto \theta^{\alpha+S_n-1} (1-\theta)^{\beta+n-S_n-1}$$

$$\Rightarrow \theta | \mathcal{D}_n \sim \text{Beta}(\alpha+S_n, \beta+n-S_n)$$

Special case: $\alpha = \beta = 1$ leads to uniform (flat) prior

Posterior
mean

$$\bar{\theta}_n = \frac{\alpha+S_n}{\alpha+\beta+n}$$

$$= \left(\frac{n}{\alpha+\beta+n} \right) \left(\frac{S_n}{n} \right) + \left(\frac{\alpha+\beta}{\alpha+\beta+n} \right) \left(\frac{\alpha}{\alpha+\beta} \right)$$

Sum to 1

ML-estimate

prior mean

Note: Conjugacy: prior & posterior belong to the same family of parameterized distributions.

e.g. Bernoulli case: Beta prior \Rightarrow conjugacy.

Example:

$$\mathcal{D}_n = \{x_1, \dots, x_n\}$$

$$f(x|\theta) \sim N(\theta, \sigma^2)$$

known

$$\text{Prior } \pi(\theta) \sim N(\theta_0, \sigma_0^2)$$

$$f(\theta | \mathcal{D}_n) \propto \left[\prod_{i=1}^n \exp\left(-\frac{1}{2} \left(\frac{x_i - \theta}{\sigma}\right)^2\right) \right] \exp\left(-\frac{1}{2} \left(\frac{\theta - \theta_0}{\sigma_0}\right)^2\right)$$

$$\propto \exp\left(-\frac{1}{2} \left[\underbrace{\sum_{i=1}^n \left(\frac{x_i - \theta}{\sigma}\right)^2}_{\text{quadratic in } \theta} + \left(\frac{\theta - \theta_0}{\sigma_0}\right)^2 \right]\right) \quad (*)$$

$$\text{So, } f(\theta | \mathcal{D}_n) \sim N(\theta_n, \sigma_n^2)$$

$$f(\theta | \mathcal{D}_n) \propto \exp\left(-\frac{1}{2} \left(\frac{\theta - \theta_n}{\sigma_n}\right)^2\right) \quad (**)$$

Equating the co-efficients of θ & θ^2 in (*) & (**)

$$\frac{1}{\sigma_n^2} = \left(\frac{n}{\sigma^2} + \frac{1}{\sigma_0^2} \right) \quad \leftarrow \text{Coeff. of } \theta^2$$

$$\frac{\theta_n}{\sigma_n^2} = \frac{n}{\sigma^2} \bar{S}_n + \frac{\theta_0}{\sigma_0^2} \quad \leftarrow \text{Co-eff. of } \theta$$

$$\Rightarrow \theta_n = \left(\frac{n \sigma_0^2}{n \sigma_0^2 + \sigma^2} \right) \left(\frac{\bar{S}_n}{n} \right) + \left(\frac{\sigma^2}{n \sigma_0^2 + \sigma^2} \right) \theta_0$$

$$\sigma_n^2 = \frac{\sigma_0^2 \sigma^2}{n \sigma_0^2 + \sigma^2}$$

Some observations:-

- ① θ_n lies between $\frac{\sum y_i}{n}$ & θ_0
- ② $\sigma_0 \neq 0 \Rightarrow \theta_n \rightarrow \frac{\sum y_i}{n}$ as $n \rightarrow \infty$
- ③ $\sigma_0 = 0 \Rightarrow$ Prior dominates
- ④ $\sigma_0 \gg \sigma \Rightarrow \theta_n \approx \frac{\sum y_i}{n}$

Ref: Duda Hart Stork's book for Bayes Classifier & ML/Bayes estimation

Minimum mean square error estimation

Ref: Sec 4.9 of
Bruce Hajek's notes
on probability
(ECE 313 UIUC)

I Constant estimators:

Y is a r.v. & we wish to estimate Y
by a constant δ .

$$\text{MSE}(\delta) = E(Y - \delta)^2$$

$$= \int_{-\infty}^{\infty} (y - \delta)^2 f_Y(y) dy$$

It is easy to see that $\delta^* = EY$ minimizes the MSE.

So, EY is the MMSE estimate.

II Unconstrained estimators

Y is a r.v. & we observe X .

$$\text{MSE} = E(Y - g(X))^2$$

↑
Want to find the g that minimizes the MSE

Suppose you observe $X=10$.

$$E[Y | X=10] = \int_{-\infty}^{\infty} y f_{Y|X}(y|x) dy$$

Claim: $E[Y | X=x]$ is the MMSE estimate

$$\text{MSE} = E[(Y - g(X))^2]$$

$$= \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} (y - g(x))^2 f_{Y|X}(y|x) dy \right] f_X(x) dx$$

minimized by \downarrow $g^*(x) = E[Y | X=x]$

$$\text{MMSE} = E \left[(Y - E[Y|X])^2 \right]$$

show that $\stackrel{2}{=} E[Y^2] - E\left[(E[Y|X])^2 \right]$

Some problems

- ① Bayes estimation, Gaussian: unknown mean
known variance σ^2

Aim: Sequential estimation of posterior mean & variance

From class notes (see above),

$$\begin{aligned} \textcircled{1} \quad \frac{1}{\sigma_n^2} &= \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2} \\ &= \frac{1}{\sigma^2} + \frac{n-1}{\sigma^2} + \frac{1}{\sigma_0^2} \\ &= \frac{1}{\sigma^2} + \frac{1}{\sigma_{n-1}^2} \end{aligned}$$

$$\begin{aligned} \textcircled{2} \quad \frac{\partial}{\sigma_n^2} &= \frac{S_n}{\sigma^2} + \frac{\partial}{\sigma_0^2} \\ &= \frac{S_{n-1}}{\sigma^2} + \frac{x_n}{\sigma^2} + \frac{\partial}{\sigma_0^2} \end{aligned}$$


$$= \frac{\sigma_{n-1}^2}{\sigma^2} + \frac{\sigma_n^2}{\sigma^2}$$

Pb 2)

$$x_1 = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \quad x_2 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad x_3 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\bar{x} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$C = \frac{1}{3} \sum_{i=1}^3 x_i x_i^T = \frac{2}{3} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

Top λ eigenvalue = $\frac{4}{3}$ & corresponding eigenvector = $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ 

$$\tilde{x}_i = (x_i^T u_1) u_1 + \cancel{(x_i^T u_2) u_2} \quad 0$$

$$\tilde{x}_1 = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \quad \tilde{x}_2 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \tilde{x}_3 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Pb 3) Linear estimator

$$\begin{aligned} \text{MSE} &= E \left[(Y - (aX + b))^2 \right] \\ &= E \left[((Y - aX) - b)^2 \right] \end{aligned}$$

So, for a given a ,

$$\begin{aligned} b &= E(Y - aX) \\ &= \mu_Y - a\mu_X \end{aligned}$$

The estimator has the form $aX + \mu_Y - a\mu_X$

$$\begin{aligned}
\text{MSE} &= E \left[(Y - \mu_Y - aX + a\mu_X)^2 \right] \\
&= E \left[\left[(Y - aX) - (\mu_Y - a\mu_X) \right]^2 \right] \\
&= \text{Var}(Y - aX) \\
&= \text{Cov}(Y - aX, Y - aX) \\
&= \text{Var}(Y) - 2a \text{Cov}(Y, X) + a^2 \text{Var}(X) \quad (*)
\end{aligned}$$

Differentiate (*) wrt a to obtain

$$a^* = \frac{\text{Cov}(Y, X)}{\text{Var}(X)}$$

$$\begin{aligned}
\text{Best linear estimator} &= L^*(X) = a^*X + b^* \\
&= a^*X + \mu_Y - a^*\mu_X
\end{aligned}$$

$$= \left(\frac{\text{Cov}(Y, X)}{\text{Var} X} \right) (X - \mu_X) + \mu_Y$$

$$= \mu_Y + \sigma_Y \rho_{X,Y} \left(\frac{X - \mu_X}{\sigma_X} \right)$$

$$\text{MMSE} = \text{Var}(Y - a^*X)$$

$$= \sigma_Y^2 - \left(\frac{\sigma_Y^2 \rho_{X,Y}^2}{\sigma_X^2} \right) \cdot \sigma_X^2$$

$$= \sigma_Y^2 (1 - \rho_{X,Y}^2)$$

Pb 4) ML estimation for Geometric (θ)

$$L(\theta) = \prod_{i=1}^n (1-\theta)^{x_i-1} \theta$$

$\{x_1, \dots, x_n\}$
 $\sum_{i=1}^n x_i = S_n$

$$= (1-\theta)^{S_n-n} \theta^n$$

$$L'(\theta) = - (1-\theta)^{S_n-n-1} (S_n-n) \theta^n + (1-\theta)^{S_n-n} n \theta^{n-1}$$

$$= (1-\theta)^{S_n-n-1} \theta^{n-1} \left[- (S_n-n) \theta + n (1-\theta) \right]$$

$$= (1-\theta)^{S_n-n-1} \theta^{n-1} \left[n - S_n \theta \right]$$

$$L' > 0 \quad \text{if} \quad n > S_n \theta \quad \text{i.e.,} \quad \theta < \frac{1}{\left(\frac{S_n}{n}\right)}$$

$$= 0 \quad \text{if} \quad \theta = \frac{1}{\left(\frac{S_n}{n}\right)}$$

$$< 0 \quad \text{if} \quad \theta > \frac{1}{\left(\frac{S_n}{n}\right)}$$

$$\text{So, } \hat{\theta}_{ML} = \frac{1}{\left(\frac{S_n}{n}\right)}$$

Pb 5)

Intuitive justification for ML estimate of variance being biased

$$E\left(\frac{1}{n} \sum_{i=1}^n (x_i - \mu)^2\right) = \sigma^2$$

Recall $\hat{\sigma}_{MC}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\mu}_n)^2$
 Observe that

$$\sum_{i=1}^n (x_i - \hat{\mu}_n)^2 \geq \sum_{i=1}^n (x_i - \mu)^2 \quad (*)$$

Why?

$$\begin{aligned} \text{RHS} &= \sum_{i=1}^n \left((x_i - \hat{\mu}_n) + (\hat{\mu}_n - \mu) \right)^2 \\ &= \sum_{i=1}^n (x_i - \hat{\mu}_n)^2 + \sum_{i=1}^n (\hat{\mu}_n - \mu)^2 + \underbrace{\text{Cross term}}_{\text{vanishes}} \\ &\geq \sum_{i=1}^n (x_i - \hat{\mu}_n)^2 \end{aligned}$$

from (*),

$$E\left(\frac{1}{n} \sum_{i=1}^n (x_i - \hat{\mu}_n)^2\right) \geq \sigma^2$$