

Topic 4. Dimension Reduction

Deterministic

(P.C.A)

Principal Component

Analysis

1) Introduction

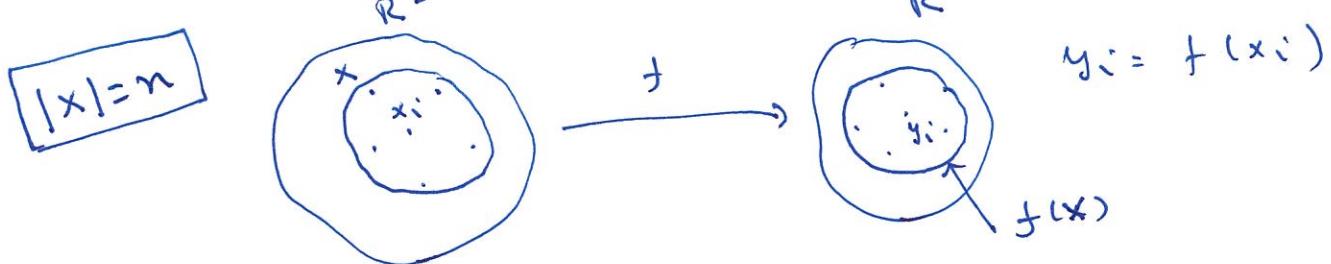
Let X be finite subset of vectors in \mathbb{R}^D , D -large

Goal is to find a mapping $f: X \subset \mathbb{R}^D \rightarrow \mathbb{R}^k$

~~such that $f(x) = \dots$~~ such that $f(x) = \dots$

$\{f(x_i) \mid x_i \in X\}$ the set of all images of $x_i \in X$

in \mathbb{R}^k have the desired property.



One property of interest is the preservation of pair-wise distances. Consider Euclidean distances

The map is said to be an isometry if

for $u, v \in X$

$$\|f(u) - f(v)\| = \|u - v\| \longrightarrow ①$$

Isometric embedding is feasible for $k \geq D$. But, for $k < D$, the best we can hope for near isometry where distances are approximately preserved.

Definition 1 $f: X \subset \mathbb{R}^D \rightarrow \mathbb{R}^k$ is called a Lipschitz map if for $u, v \in X$ and constants A and B the following holds:

$$A \|u - v\|^2 \leq \|f(u) - f(v)\|^2 \leq B \|u - v\|^2 \rightarrow ②$$

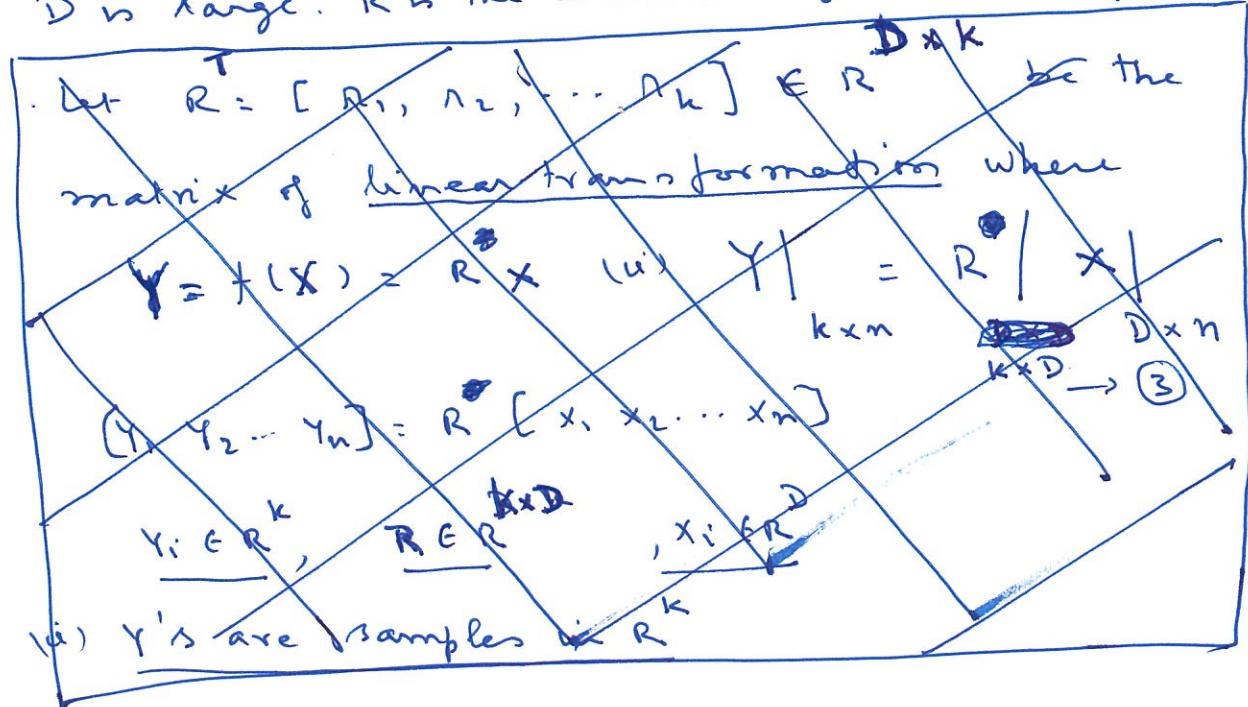
(ii) distances are approximately preserved.

- Methods to realize Lipschitz map is not easy and it is here random projections come into the picture.

- It is shown below that the map that approximately preserve the distance can be realized as a linear map defined by random projection matrix

2) Random Projection: Let $X \subset \mathbb{R}^D$ (ii) $X \in \mathbb{R}^{D \times n}$

matrix where the n elements are the n columns of the given data matrix where D is large. k is the dimension of the target space.



(3)

- Let $R \in \mathbb{R}^{k \times D}$ matrix of linear transformation of interest to realize the Lipschitz map that is very near isometry.

- Define $x = [x_1, x_2, \dots, x_n] \quad x_i \in \mathbb{R}^D$
 $y = [y_1, y_2, \dots, y_n] \quad y_i \in \mathbb{R}^k$

- Define $y = R|x| \quad \xrightarrow{\text{3}}$

where $R = [r_{is}] \quad 1 \leq i \leq k, 1 \leq s \leq D$

maps the vector $x_i \in \mathbb{R}^D$ to $y_i \in \mathbb{R}^k$ for $1 \leq i \leq n$ and $k \ll D$.

Note: When we realize τ as a linear map, it is computationally simpler to implement.

Notice x is used to denote the set of n points in \mathbb{R}^D as well as the matrix of size $D \times n$ where each vector is a column.

x represents the given configuration of data in \mathbb{R}^D and Y is the embedded configuration in \mathbb{R}^k

Our goal is to preserve the local separation approximately.

Two questions arise: How to pick the elements of the matrix $R \in \mathbb{R}^{k \times D}$? Prove that such a choice can indeed realize near isometric embedding of $X \subset \mathbb{R}^D$ in \mathbb{R}^k for $k \ll D$.

There are various choices for the elements of R .

Let r_{ij} be the typical element of R
 $1 \leq i \leq k, 1 \leq j \leq D$. There are three types

1) $r_{ij} \sim N(0, 1)$ i.i.d samples

Types
2) $r_{ij} \in \{-1, 1\}$ with probability $\frac{1}{2}$ each

3) $r_{ij} \in \{\pm \sqrt{3}, 0\}$: $r_{ij} = \pm \sqrt{3}$ with prob. = $\frac{1}{6}$
= 0 with prob = $\frac{2}{3}$

In each case, verify

$$E[r_{ij}] = 0, \text{ var}(r_{ij}) = 1$$

The random matrix R is said to be of Type 1, 2, 3 if r_{ij} is of type 1, 2, 3 respectively.

The action of R is defined as follows.

If $N = f(u)$, then

$$N = \boxed{f(u)} = \frac{1}{\sqrt{k}} RU \quad \rightarrow (4)$$

(ii) the D vectors in X are mapped to k vectors in Y .

The set Y is called the random projection of X .

Property 1: Let $R \in \mathbb{R}^{K \times D}$ matrix with its elements being i.i.d random variables with zero mean and unit variance. Then the map $f: \mathbb{R}^D \rightarrow \mathbb{R}^K$ defined by

$$\textcircled{f}(a) = \frac{1}{\sqrt{k}} Ra, \quad a \in \mathbb{R}^D. \rightarrow \textcircled{5}$$

Then $f(a)$ is a random vector in \mathbb{R}^K whose components are ~~i.i.d~~ random variables with mean zero and Variance $\frac{1}{k} \|a\|^2$. That is

$$\boxed{\textcircled{5}} \quad E[\|f(a)\|^2] = \|a\|^2 \rightarrow \textcircled{6}.$$

Proof: Let r_i be the i^{th} row vector of R .

Then the inner product $\langle r_i, a \rangle = c_i$

Then, $c = (c_1, c_2, \dots, c_k)^T$ is given by

$$c = f(a) = \frac{1}{\sqrt{k}} Ra \quad \textcircled{5}$$

$$\cdot \quad E(c_i) = \frac{1}{\sqrt{k}} \sum_{j=1}^D E[R_{ij}; a_j]$$

$$= \frac{1}{\sqrt{k}} \sum_{j=1}^D a_j E[R_{ij}] = 0$$

$$\cdot \quad E[c_i c_j] = \frac{1}{k} \sum_{m=1}^k \sum_{i=1}^D a_m a_j E[r_{im} r_{mj}]$$

$$= 0 \quad \text{for } i \neq j$$

$$\cdot \quad E[c_i^2] = \frac{1}{k} E \left[\left(\sum_{j=1}^D a_j r_{ij} \right)^2 \right]$$

$$= \frac{1}{k} \left[\sum_{j=1}^D a_j^2 E[r_{ij}^2] + \right.$$

$$\left. 2 \sum_{i \neq m} a_i a_m E[r_{ij}] E[r_{im}] \right]$$

r_{ij} are i.i.d

$$E(r_{ij}) = 0 \quad E(r_{ij}^2) = 1$$

(6)

$$= \frac{1}{k} \sum_{j=1}^D a_j^2 = \frac{1}{k} \|a\|^2$$

~~DEFINITION~~

$$\begin{aligned}\therefore E[\|c\|^2] &= E[\|(f(a))\|^2] = E\left[\sum_{i=1}^D c_i^2\right] \\ &= \sum_{i=1}^D E(c_i^2) \\ &= k \cdot \frac{1}{k} \|a\|^2 = \|a\|^2.\end{aligned}$$

This result holds good for all three types of matrices described above.

Property 2: Let f be a map as in Property 1.

Let $a \in \mathbb{R}^D$ be a unit vector. Then $\sum_k f(a)$ is a random vector in \mathbb{R}^K whose entries are i.i.d.r.v. with mean zero and unit variance.

Remarks:

1) The matrix $R \in \mathbb{R}^{D \times K}$ has non-trivial null space: $N(R) = \{u \in \mathbb{R}^D : Ru = 0\}$. Hence, the set X of points cannot be totally ~~arbitrary~~ arbitrary. So on a given sub-set we need to justify that Lipschitz embedding exists.

2) Johnson-Lindenstrauss first proved the following:

J-L lemma (1981): Let $\epsilon > 0$ and n , an integer be given. Then for all integers $k \geq k_0 = O(\epsilon^{-2} \log n)$ and a set X of n points

(7)

randomly selected in \mathbb{R}^D , there exists a $f: \mathbb{R}^D \rightarrow \mathbb{R}^k$ which satisfies

$$(1-\varepsilon) \|u-v\|^2 \leq \|f(u) - f(v)\|^2 \leq (1+\varepsilon) \|u-v\|^2$$

$\rightarrow (7)$

for all $u, v \in X$.

- The f in J-L lemma is called J-L embedding.
- J-L did not give lower bound on k .
- It was made clear subsequently that f can be realized using random projection.
- Various lower bounds on k were subsequently established.

3) Random Projection based on Gaussian Variables

Theorem 1:- Dasgupta and Gupta (1999) For any $\varepsilon > 1$ and integer $n > 0$, let k be a positive integer such that-

$$k \geq 4 \left[\frac{\varepsilon^2}{2} + \frac{\varepsilon^3}{3} \right]^{-1} \log n. \rightarrow (8)$$

Then for any set $X \subset \mathbb{R}^D$ of n -points, there is a linear map, $f: \mathbb{R}^D \rightarrow \mathbb{R}^k$ such that for all $u, v \in X$

$$(1-\varepsilon) \|u-v\|^2 \leq \|f(u) - f(v)\|^2 \leq (1+\varepsilon) \|u-v\|^2$$

$\rightarrow (9)$

Furthermore, this map can be found in

$\log n = \ln n$
natural log

random polynomial time.

Note:- An algorithm has randomized polynomial time if it runs in polynomial time (in input size) and, if the correct answer is No, it always returns No, while the correct answer is Yes, it returns Yes with a positive probability.

- The proof of this theorem depends on a

Lemma 2: Let $R \in \mathbb{R}^{k \times D}$ random matrix of Type 1 and let $a \in \mathbb{R}^D$ be a unit vector.

~~Let~~ $y = Ra$ and $\beta > 1$. Then

$$P_r \left[\|y\|^2 \leq \frac{k}{\beta} \right] \leq \exp \left[\frac{k}{2} \left(1 - \frac{1}{\beta} - \ln \beta \right) \right] \rightarrow (9)$$

and

$$P \left[\|y\|^2 \geq \frac{k\beta}{\beta} \right] \leq \exp \left[\frac{k}{2} \left(1 - \frac{1}{\beta} + \ln \beta \right) \right] \rightarrow (10)$$

Note:-

- These are related to Concentration results.

- First let us take this lemma for granted and use it to prove the Theorem 1.
- We will come back later to ~~prove~~ prove this lemma 2.

ln = natural log

(9)

- Proof of Theorem 1: Recall R is a $K \times D$ matrix with i.i.d. elements from $N(0, 1)$.
- Let $u, v \in X$ be two distinct elements of X , and let $a = \frac{u-v}{\|u-v\|}$. Let $f(a) = \frac{1}{\sqrt{k}} Ra$.
 - Define $z = f(a)$ and $y = \sqrt{k} z = Ra$

~~Then $\|f(u) - f(v)\| = \|f(a)\|$~~ Then,

$$\begin{aligned}\|z\|^2 &= \|f(a)\|^2 = \left\| f\left(\frac{u-v}{\|u-v\|}\right) \right\|^2 \\ &= \left\| \frac{1}{\sqrt{k}} R \left(\frac{u-v}{\|u-v\|} \right) \right\|^2 \\ &= \frac{1}{\|u-v\|^2 k} \|R(u-v)\|^2 \rightarrow (11)\end{aligned}$$

Now $f(u) = \frac{1}{\sqrt{k}} Ru$, $f(v) = \frac{1}{\sqrt{k}} Rv$

$$\begin{aligned}f(u) - f(v) &= \frac{1}{\sqrt{k}} R(u-v) \\ \Rightarrow \|f(u) - f(v)\|^2 &= \frac{1}{k} \|R(u-v)\|^2 \rightarrow (12)\end{aligned}$$

Combining (11) and (12):

$$\|z\|^2 = \frac{\|f(u) - f(v)\|^2}{\|u-v\|^2} \rightarrow (13)$$

Thus

$$\begin{aligned}P\left[\frac{\|f(u) - f(v)\|^2}{\|u-v\|^2} \leq 1-\varepsilon\right] &= P[\|z\|^2 \leq 1-\varepsilon] \\ &= P[\|y\|^2 \leq k(1-\varepsilon)] \\ &\rightarrow (14)\end{aligned}$$

(1D)

• Likewise (please verify)

$$P \left[\frac{\|f(u) - f(N)\|^2}{\|u - N\|^2} \geq 1 + \varepsilon \right] = P [\|y\|^2 \geq k(1 + \varepsilon)] \rightarrow (15)$$

Part 2: Now set $\frac{1}{\beta} = 1 - \varepsilon$ in Lemma 2 and apply to the right-hand-side of (14) to get (using (9))

$$P[\|y\|^2 \leq (1 - \varepsilon)k] \leq \exp \left[+\frac{k}{2} [1 - (1 - \varepsilon) + \ln(1 - \varepsilon)] \right] \rightarrow (16)$$

• Recall: $\log(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} \dots$ for $-1 < x \leq 1$

$$\Rightarrow \log(1-x) = -x - \frac{x^2}{2} - \frac{x^3}{3} - \frac{x^4}{4} \dots$$

$$\leq -x - \frac{x^2}{2} \quad \rightarrow (17)$$

• Apply to the exponent on the r.h.s. of (16)

$$1 - (1 - \varepsilon) + \ln(1 - \varepsilon)$$

$$\leq 1 - 1 + \varepsilon - \varepsilon - \frac{\varepsilon^2}{2} = -\frac{\varepsilon^2}{2} \quad \rightarrow (18)$$

• Combining (16) - (18):

$$P[\|y\|^2 \leq (1 - \varepsilon)k] \leq \exp \left[-\frac{k\varepsilon^2}{2} \right] \rightarrow (19)$$

Part 2: Now set $\beta = 1 + \varepsilon$ in Lemma 2 and apply it to the r.h.s. of (15) [using (10)]

$$P[\|y\|^2 \geq k(1 + \varepsilon)] \leq \exp \left[+\frac{k}{2} (1 - (1 + \varepsilon) + \ln(1 + \varepsilon)) \right]$$

The exponent becomes: $\log(1 + \varepsilon) \leq \varepsilon - \frac{\varepsilon^2}{2} + \frac{\varepsilon^3}{3} \rightarrow (20)$

$$\boxed{\cancel{\frac{k}{2}} \cancel{1 - 1 - \varepsilon + \varepsilon - \cancel{\varepsilon^2} \cancel{\frac{\varepsilon^3}{2}} \cancel{- \frac{\varepsilon^4}{4}} \dots}}$$

Then

$$\begin{aligned}
 & \frac{k}{2} [1 - (1+\varepsilon) + \ln(1+\varepsilon)] \\
 & \leq \frac{k}{2} \left[1 - 1 - \varepsilon + \varepsilon - \frac{\varepsilon^2}{2} + \frac{\varepsilon^3}{3} \right] \\
 & = \frac{k}{2} \left[-\frac{\varepsilon^2}{2} + \frac{\varepsilon^3}{3} \right]
 \end{aligned}
 \quad \rightarrow (22)$$

Combining (20) - (22) =>

$$P[|y|^2 \geq k(1+\varepsilon)] \leq e^{-\frac{k}{2} \left[\frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{3} \right]}$$

$\rightarrow (23)$

Now Consider the r. h. s. of (19) and (22):

Recall: $\frac{k}{2} \varepsilon^2 \geq \frac{k}{2} \left[\frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{3} \right]$

$$\Rightarrow -\frac{k}{2} \varepsilon^2 \leq -\frac{k}{2} \left[\frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{3} \right]$$

$$\Rightarrow \exp \left[-\frac{k}{2} \varepsilon^2 \right] \leq \exp \left[-\frac{k}{2} \left(\frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{3} \right) \right] \rightarrow (24)$$

Hence, set

$$\exp \left[-\frac{k}{2} \left(\frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{3} \right) \right] \leq \exp[-2 \ln n] \rightarrow (25)$$

This inequality (25) is true when

$$-\frac{k}{2} \left(\frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{3} \right) \leq 2 \log n$$

$$\Rightarrow \frac{k}{2} \left(\frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{3} \right) \geq -2 \log n$$

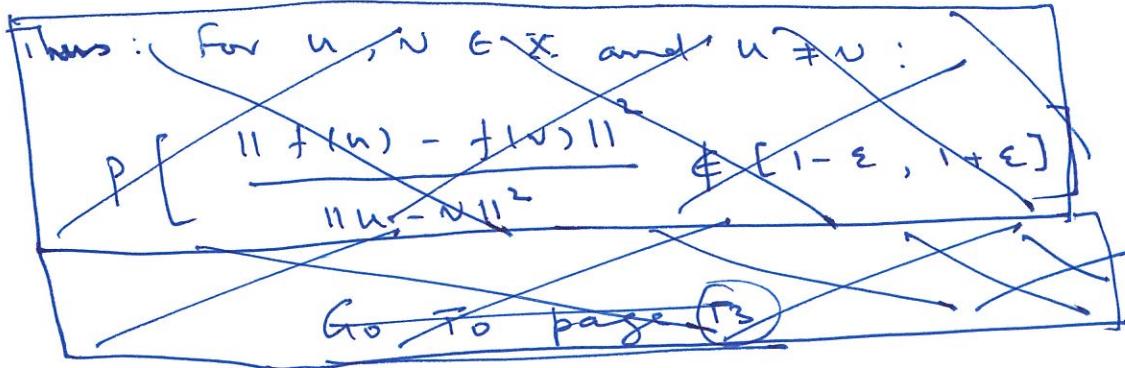
$$\Rightarrow k \geq \frac{4 \log n}{\left[\frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{3} \right]} \quad \text{only when } \frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{3} > 0$$

$\rightarrow (26)$

This applies to (20) and (23) simultaneously.

Thus, when k satisfies (26) :

$$\exp[-2\log_e n] = e^{-2\ln n} = e^{-\log_e n^2} \\ = e^{\log\left(\frac{1}{n^2}\right)} = \frac{1}{n^2} \rightarrow (27)$$



- So by (24) this bound applies to the r.h.s. of (19) and (23). Hence from (19) and (23) we get

$$P\left[\frac{\|y\|^2}{k} \leq (1-\varepsilon)\right] \leq \frac{1}{n^2}$$

and

$$P\left[\frac{\|y\|^2}{k} \geq (1+\varepsilon)\right] \leq \frac{1}{n^2}$$

$$\begin{aligned} P[A \cup B] \\ \leq P[A] + P[B] \end{aligned}$$

- Then

$$P\left[\frac{\|y\|^2}{k} \notin [1-\varepsilon, 1+\varepsilon]\right] \leq \frac{2}{n^2} \rightarrow (28)$$

- Hence, from

$$\frac{\|y\|^2}{k} = \frac{\|f(u) - f(v)\|^2}{\|u - v\|^2} \rightarrow (29)$$

we get that for each pair u, v and $u \neq v$,

$$(1-\varepsilon)\|u - v\|^2 \leq \|f(u) - f(v)\|^2 \leq (1+\varepsilon)\|u - v\|^2$$

holds with probability at least $(1 - \frac{2}{n^2})$

?

(13)

Lemma 2 :- Let $R \in \mathbb{R}^{k \times D}$ random matrix of Type 2 and let $a \in \mathbb{R}^D$ be a unit vector. Let $y = Ra$ and $\beta > 1$. Then

$$P[||y||^2 \leq \frac{k}{\beta}] < \exp \left[\frac{k}{2} \left(1 - \frac{1}{\beta} - \ln \beta \right) \right] \rightarrow (9)$$

and

$$P[||y||^2 \geq k\beta] < \exp \left[\frac{k}{2} \left(1 - \beta + \ln \beta \right) \right] \rightarrow (10)$$

Proof :- Consider (9):

$$\cdot P[||y||^2 \leq \frac{k}{\beta}] = P[\exp(-h||y||^2) \geq \exp(-\frac{kh}{\beta})]$$

$$\xrightarrow{\text{(Markov inequality)}} \leq E[\underbrace{\exp(-h||y||^2)}_{I}] \exp \left[\frac{kh}{\beta} \right] \rightarrow (30)$$

Want to find the min. value of r.h.s of (30)

Compute I :-

$$\cdot y = R[a] \Rightarrow y_i = \sum_{j=1}^D n_{ij} a_j - \text{Linear combination of } n_{ij}$$

$$\cdot n_{ij} \sim i.i.d N(0, 1), \Rightarrow y_i \text{ is Normal}$$

$$\begin{aligned} \cdot E(y_i) &= 0 \text{ and } E(y_i^2) = \text{Var}(y_i) \\ &= \sum E(n_{ij}^2) a_j^2 \\ &= \sum a_j^2 = 1 \end{aligned} \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} (31)$$

$$\cdot E[y^T y] = E\left(\sum_{i=1}^k y_i^2\right) = \sum_{i=1}^k E(y_i^2) = k$$

$$\begin{aligned} \therefore E[\exp(-h y_i^2)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-hy_i^2} e^{-\frac{y_i^2}{2}} dy_i \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-y_i^2 [h + \frac{1}{2}]} dy_i \end{aligned} \quad \rightarrow (31)$$

(14)

$$\begin{aligned}
 \text{But } e^{-y_i^2(h + \frac{1}{2})} &= e^{-y_i^2 \frac{[2h+1]}{2}} \\
 &= e^{-\frac{y_i^2}{2 \cdot \frac{1}{1+2h}}} = e^{-\frac{y_i^2}{2a^2}}
 \end{aligned}$$

$$\therefore E[\exp(-hy_i^2)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{y_i^2}{2a^2}} dy_i$$

$$= a \cdot \frac{1}{\sqrt{2\pi} a} \int_{-\infty}^{\infty} e^{-\frac{y_i^2}{2a^2}} dy_i$$

$$= a = \frac{1}{\sqrt{1+2h}} \rightarrow (32)$$

Hence, from (30): Combining (30), (31) and (32)

$$\begin{aligned}
 E\left[\exp\left[-h\|y\|\right]^2\right] \exp\left[\frac{hk}{\beta}\right] \\
 = \left(\frac{1}{\sqrt{1+2h}}\right)^k \exp\left[\frac{hk}{\beta}\right] = (1+2h)^{-\frac{k}{2}} \exp\left[\frac{hk}{\beta}\right]
 \end{aligned}$$

$$\rightarrow (33)$$

$$\text{Define } g(h) = (1+2h)^{-\frac{k}{2}} \exp\left[\frac{hk}{\beta}\right] \quad h > 0$$

$$\rightarrow (34)$$

I.H.W.L. Verify that $g(h)$ attains a min. value at $h^* = \frac{\beta-1}{2}$. Then, from (34):

$$\Rightarrow g(h^*) = \beta^{-\frac{k}{2}} \exp\left[\frac{k}{2}(1-\beta)\right] \rightarrow (35)$$

Recall: $a = e^{\ln a}$ for $a > 0 \rightarrow (36)$

Thus: $\beta = e^{\ln \beta (-k/2)}$

$$= e^{-\frac{k}{2} \ln \beta} \quad \rightarrow (37)$$

• Substitute (37) in (35):

$$\min \text{val} \{ g(h) \} = g(h^*) = e^{-\frac{k}{2} \ln \beta}$$

$$= \exp \left[-\frac{k}{2} (1 - \beta - \ln \beta) \right]$$

• Then

$$g(h^*) = e^{-\frac{k}{2} \ln \beta} = e^{\frac{k}{2} [1 - \beta]}$$

$$= \exp \left[\frac{k}{2} (1 - \beta - \ln \beta) \right] \rightarrow (38)$$

(ii) The min. value of the r. h. s. of (30) is given by (38) which is the claim ~~(19)~~ in Lemma 2.

Now, consider (10)

$$P [\|y_1\|^2 \geq k\beta] = P [\exp (h \|y_1\|^2) \geq \exp (hk\beta)]$$

Markov's inequality

$$\leq E[\exp (h \|y_1\|^2)] \exp [-hk\beta] \rightarrow (39)$$

• Verify by the above argument that

$$E[\exp (h \|y_1\|^2)] = \frac{1}{\sqrt{1-2h}} \begin{cases} (0 < h < \frac{1}{2}) \\ \rightarrow (40) \end{cases}$$

$$E[\exp (h \|y_1\|^2)] = (1-2h)^{-k/2}$$

$$\therefore P[||y||^2 \geq k\beta] \leq (1-2h)^{-\frac{k}{2}} \exp[-h k \beta]$$

Define $g(h) = (1-2h)^{-\frac{k}{2}} \exp[-h k \beta]$

$g(h)$ attains its min. at $h^* = \frac{\beta-1}{2\beta}$

and $g(h^*) = \beta^{\frac{k}{2}} \exp\left[-\frac{k}{2}(\beta-1)\right]$

$$= \exp\left[-\frac{k}{2}(\beta-1) + \frac{h}{2} \ln \beta\right]$$

$$= \exp\left[\frac{k}{2}(1-\beta - \ln \beta)\right] \rightarrow (41)$$

which proves (iv).

This concludes the proof of the theorem.

∴