Lecture 10: $\left\{\begin{array}{l}\text{Karhunen-Loève Transform}\\ \text{Principal Component Analysis}\end{array}\right.$

Note Title 2/3/2014

Consider a stochastic process in $\mathbb{C}^n$ s.t.

R.V.: upper-case

$\mathbf{X} \in \mathbb{C}^n \sim f_{\mathbf{X}}(x_1, \cdots, x_n)$ pdf.

[random vector, i.e., each coordinate is a r.v. (or random signal)

Now consider its covariance :

$$\Gamma_{\mathbf{X}}[k,\ell] := \underset{\sim}{E}\left[(X_k - \underset{\sim}{E}X_k)\overline{(X_\ell - \underset{\sim}{E}X_\ell)}\right]$$

↳ expectation $k, \ell = 1:n$

i.e., $\Gamma_{\mathbf{X}} := E(\mathbf{X} - E\mathbf{X})(\mathbf{X} - E\mathbf{X})^*$

$$= E\,\mathbf{X}\mathbf{X}^* - (E\mathbf{X})(E\mathbf{X})^* \in \mathbb{C}^{n\times n}$$

Realizations (obs.'s) ⇒ lower-case

Let $\{\mathbf{x}_1, \cdots, \mathbf{x}_N\}$ be N realizations of $\mathbf{X}$. Then, the sample estimate of $\Gamma_{\mathbf{X}}$ is:

$$\hat{\Gamma}_{\mathbf{X}} := \frac{1}{N}\sum_{j=1}^{N} \mathbf{x}_j \mathbf{x}_j^* - \bar{\mathbf{x}}\bar{\mathbf{x}}^*$$

where $\bar{\mathbf{x}} := \frac{1}{N}\sum_{j=1}^{N} \mathbf{x}_j$

<u>If</u> we define the data matrix

$$X := [\mathbf{x}_1 | \mathbf{x}_2 | \cdots | \mathbf{x}_N] \in \mathbb{C}^{n\times N},$$

<u>then</u> $\hat{\Gamma}_{\mathbf{X}} = \frac{1}{N} X X^* - \bar{\mathbf{x}}\,\bar{\mathbf{x}}^*.$

Suppose we want a <u>data-adaptive</u> ONB of $\mathbb{C}^n$ (unlike fixed ONBs such as DFT, DCT, DST) s.t. the realizations of this stochastic process as a whole (i.e., <u>on average</u>) can be best approximated by m coordinates with $\underline{m \ll n}$ in the mean-squared (L^2) error sense.

Let $W \in U(n) :=$ a set of all unitary matrices in $\mathbb{C}^n$ and let $\mathbb{Y} = W^* \mathbb{X}$.

$\Rightarrow$ viewing $\mathbb{X}$ relative to W (or the ONB consisting of col's of W)

$\mathbb{X}$ is viewed relative to I_n.

$$\Rightarrow \mathbb{X} = W\mathbb{Y} = [w_1 | \cdots | w_n] \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix}$$

$$= [e_1 | \cdots | e_n] \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix}$$

$$= Y_1 w_1 + \cdots + Y_n w_n.$$

Suppose we retain $Y_1 \sim Y_m$ and replace $Y_{m+1} \sim Y_n$ by $\alpha_{m+1} \sim \alpha_n$ (predetermined val's). Then the approx. of $\mathbb{X}$ is given by

$$\mathbb{X}^{(m)} := \sum_{j=1}^{m} Y_j w_j + \sum_{j=m+1}^{n} \alpha_j w_j$$

The error is $\Delta \mathbb{X} := \mathbb{X} - \mathbb{X}^{(m)} = \sum_{j=m+1}^{n} (Y_j - \alpha_j) w_j$, and the mean-squared error is

$$\mathcal{E}(m) := E \|\Delta \mathbb{X}\|^2 = E (\Delta \mathbb{X})^* (\Delta \mathbb{X})$$

$$= E \left[\sum_{j=m+1}^{n} \sum_{k=m+1}^{n} \overline{(Y_j - \alpha_j)} (Y_k - \alpha_k) \underbrace{w_j^* w_k}_{= \delta_{jk}} \right]$$

$$= E \left[\sum_{j=m+1}^{n} |Y_j - \alpha_j|^2 \right]$$

Step 1. $\dfrac{\partial \mathcal{E}^{(m)}}{\partial \alpha_j} = -2E(\mathbb{Y}_j - \alpha_j) = 0, \ j = m+1 : n.$

$\Rightarrow \ \alpha_j = E\mathbb{Y}_j = E[w_j^* \mathbb{X}] = w_j^* E[\mathbb{X}].$

Then, $\mathcal{E}(m) = E\left[\sum_{j=m+1}^{n} (\mathbb{Y}_j - \alpha_j)\overline{(\mathbb{Y}_j - \alpha_j)}\right]$

$$= \sum_{j=m+1}^{n} E\, w_j^*(\mathbb{X} - E\mathbb{X})\left(w_j^*(\mathbb{X} - E\mathbb{X})\right)^*$$

$$= \sum_{j=m+1}^{n} E\, w_j^*(\mathbb{X} - E\mathbb{X})(\mathbb{X} - E\mathbb{X})^* w_j$$

$$= \sum_{j=m+1}^{n} w_j^* E(\mathbb{X} - E\mathbb{X})(\mathbb{X} - E\mathbb{X})^* w_j$$

$$= \sum_{j=m+1}^{n} w_j^* \Gamma_{\mathbb{X}} w_j$$

Step 2. What kind of $\{w_j\}$ minimizes the above quantity subject to $w_j^* w_j = 1$.

$\Rightarrow$ Use the Lagrange multiplier:

$$\tilde{\mathcal{E}}(m) := \mathcal{E}(m) - \sum_{j=m+1}^{n} \lambda_j (w_j^* w_j - 1)$$

$$= \sum_{j=m+1}^{n} \left[w_j^* \Gamma_{\mathbb{X}} w_j - \lambda_j (w_j^* w_j - 1) \right]$$

$$\frac{\partial \tilde{\mathcal{E}}(m)}{\partial w_j} = 2\Gamma_{\mathbb{X}} w_j - 2\lambda_j w_j = 0$$

$\Rightarrow \ \Gamma_{\mathbb{X}} w_j = \lambda_j w_j$ Eigenvalue problem!

$1 \le m \le n$ was arbitrary. So, for any $1 \le m \le n$, we need to solve $\Gamma_{\mathbb{X}} w_j = \lambda_j w_j$, $j = 1 : m$.

$\Gamma_{\mathbb{X}}$: hermitian → unitarily diagonalizable & $\lambda_j \in \mathbb{R}$.

Remarks

(1) In practice, $\hat{\Gamma}_X$ is used for Γ_X. The quality of $\hat{\Gamma}_X$ depends on $n > N$ or $n < N$.

$$\begin{cases} \text{classical setting: } n \ll N \text{ (e.g., census)} \Rightarrow \hat{\Gamma}_X : \text{good} \\ \text{neoclassical setting: } n \gg N \text{ (e.g., images)} \Rightarrow \hat{\Gamma}_X : \text{poor} \end{cases}$$

(2) "Only" optimal interms of the mean-squared (or the entropy) criterion.

Satosi Watanabe (1965): The Entropy Minimization Criterion.

Define $\delta_X := \mathrm{diag}(\Gamma_X) / \| \mathrm{diag}(\Gamma_X) \|_1 \in \mathbb{R}^n$

Consider all possible $W \in U(n)$ and the coordinate transf's $W^* X$.

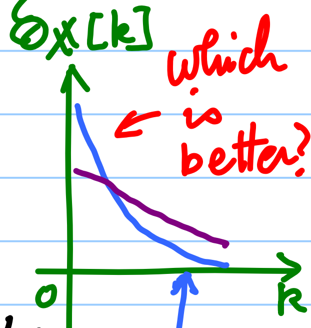
Define $H(\mathbb{p}) := \underbrace{-\sum_{i=1}^{n} p_i \log p_i}_{\text{the Shannon entropy}}$, $p_i \geq 0$, $\sum_i^n p_i = 1$.

δ_X above qualifies as $\mathbb{p}$ thanks to the normalization.

Then Watanabe showed that

$$H(\delta_{W_{KL}^* X}) = \min_{W \in U(n)} H(\delta_{W^* X})$$

i.e., $$W_{KL} = \arg\min_{W \in U(n)} H(\delta_{W^* X}).$$



That is, the KLT (or PCA) provides the minimum entropy coordinates (sharper distribution!)

⇒ Packing more energy (or variance) into the first few coordinates!

(3) $\mathbb{Y} = W_{KL}^{*} \mathbb{X}$, $W_{KL} = [\boldsymbol{w}_1 | \cdots | \boldsymbol{w}_n]$ eigenvectors of $\Gamma_{\mathbb{X}}$.

Then, what about $\Gamma_{\mathbb{Y}}$?

$$\begin{aligned}
\Gamma_{\mathbb{Y}} &= E(\mathbb{Y} - E\mathbb{Y})(\mathbb{Y} - E\mathbb{Y})^{*} \\
&= E\, W_{KL}^{*}(\mathbb{X} - E\mathbb{X})(\mathbb{X} - E\mathbb{X})^{*} W_{KL} \\
&= W_{KL}^{*}\, E(\mathbb{X} - E\mathbb{X})(\mathbb{X} - E\mathbb{X})^{*} W_{KL} \\
&= W_{KL}^{*}\, \Gamma_{\mathbb{X}}\, W_{KL} = \underline{\operatorname{diag}(\lambda_1, \cdots, \lambda_n)}
\end{aligned}$$

$$\Gamma_{\mathbb{X}} \boldsymbol{w}_j = \lambda_j \boldsymbol{w}_j, \quad \lambda_j > 0.$$

$\Rightarrow$ The components of $\mathbb{Y}$ are decorrelated!

$$E(Y_i - EY_i)\overline{(Y_j - EY_j)} = \lambda_i \delta_{ij}$$

☆ Relationship between KLT/PCA and SVD

For simplicity, let's consider the centered data matrix $\tilde{X}$ of $X \in \mathbb{C}^{n \times N}$

$$\tilde{X} := X - \frac{1}{N} X \mathbb{1}\mathbb{1}^{T} = X \underbrace{\left(I - \frac{1}{N}\mathbb{1}\mathbb{1}^{T}\right)}_{\text{centering matrix}}$$

where $\mathbb{1} := (1, 1, \cdots, 1)^{T} \in \mathbb{R}^{N}$.

Note $\bar{\mathbb{X}} = \frac{1}{N} X \mathbb{1}$, so multiplying the centering matrix from right subtracts $\bar{\mathbb{X}}$ from each col. vector $\mathbb{X}_j$ of X, $j = 1, \cdots, N$.

⇒ The mean of the col. vectors of $\tilde{X} = 0$.

Let the Singular Value Decomposition (SVD) of $\tilde{X}$ be $\tilde{X} = U \Sigma V^*$ (full SVD)

where $U \in \mathcal{U}(n) \subset \mathbb{C}^{n\times n}$

$V \in \mathcal{U}(N) \subset \mathbb{C}^{N\times N}$

$\Sigma \in \mathbb{R}^{n\times N}$: diagonal $\sigma_1, \cdots, \sigma_{\min(n,N)}$

$$\Sigma = n\left[\underbrace{\begin{matrix}\sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_{r_0} & & \\ & & & \ddots & \\ & & & & 0\end{matrix}}_{n} \;\middle|\; \underbrace{\begin{matrix} \\ \\ O \\ \\ \\ \end{matrix}}_{N-n}\right] \text{ or } \begin{array}{r} N\left\{\begin{matrix} \\ \\ \\ \\ \\ \end{matrix}\right. \\ n-N\left\{\begin{matrix} \\ \end{matrix}\right. \end{array} \underbrace{\left[\begin{array}{c} \begin{matrix}\sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_{r_0} & & \\ & & & \ddots & \\ & & & & 0\end{matrix} \\ \hline O \end{array}\right]}_{N}$$

$n < N$ classical $\qquad$ $n > N$ neoclassical

$$r = \operatorname{rank}(\tilde{X}) \leq \min(n, N-1).$$

Note that if $\{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N\}$ are linearly independent, then $\operatorname{rank}(X) \leq \min(n, N)$. However, in the case of its centered version $\tilde{X} = [\tilde{\boldsymbol{x}}_1 | \cdots | \tilde{\boldsymbol{x}}_N]$, $\tilde{\boldsymbol{x}}_j : \boldsymbol{x}_j - \bar{\boldsymbol{x}}$, $j = 1:N$, its column vectors are not linearly indep. because $\tilde{\boldsymbol{x}}_1 + \cdots + \tilde{\boldsymbol{x}}_N = 0$.

$$\Rightarrow \quad \operatorname{rank}(\tilde{X}) \leq \min(n, N-1).$$

(1) If $n < N$, then

$$\hat{\Gamma}_{\tilde{X}} = \frac{1}{N}\tilde{X}\tilde{X}^* = \frac{1}{N}U\Sigma V^* V \Sigma^* U^*$$

$$= \frac{1}{N}U\Sigma\Sigma^* U^*$$

$$= U\begin{bmatrix}\sigma_1^2/N & & 0\\ & \ddots & \\ 0 & & \sigma_n^2/N\end{bmatrix}U^* \Rightarrow$$ The eigenvalue decomposition of $\hat{\Gamma}_{\tilde{X}}$!!

Hence, in this case

$$U = W_{KL} \quad !$$

(2) If $n > N$, then we should not compute all n KLB vectors because $\mathrm{rank}(\tilde{X}) \leq N-1$, so computing more than $N-1$ KLB vectors is useless. Moreover n could be huge.

$\Rightarrow$ How to compute the top $N-1$ KLB vec's?

The first $N-1$ column vectors of $\tilde{X}V \in \mathbb{C}^{n\times N}$ = the top $N-1$ KLB vectors!

why? $\hat{\Gamma}_{\tilde{X}} = \frac{1}{N}\tilde{X}\tilde{X}^*$

so, $$\hat{\Gamma}_{\tilde{X}}\tilde{X}V = \frac{1}{N}\tilde{X}\tilde{X}^* X V$$

$$= \frac{1}{N}\tilde{X}(V\Sigma^* U^* U \Sigma V^*)V$$

$$= \frac{1}{N}\tilde{X} V \underbrace{\Sigma^*\Sigma}_{N\times N \text{ diagonal!}} = \tilde{X} V \begin{bmatrix} \sigma_1^2/N & & & 0 \\ & \ddots & & \\ & & \sigma_{N-1}^2/N & \\ 0 & & & 0 \end{bmatrix}$$

$\Rightarrow$ Each column vector of $\tilde{X}V$ is a linear combination of the column vectors of $\tilde{X}$, i.e., belongs to $\underset{\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim}{\text{span}\{\tilde{X}_1, \cdots, \tilde{X}_N\}}$!!

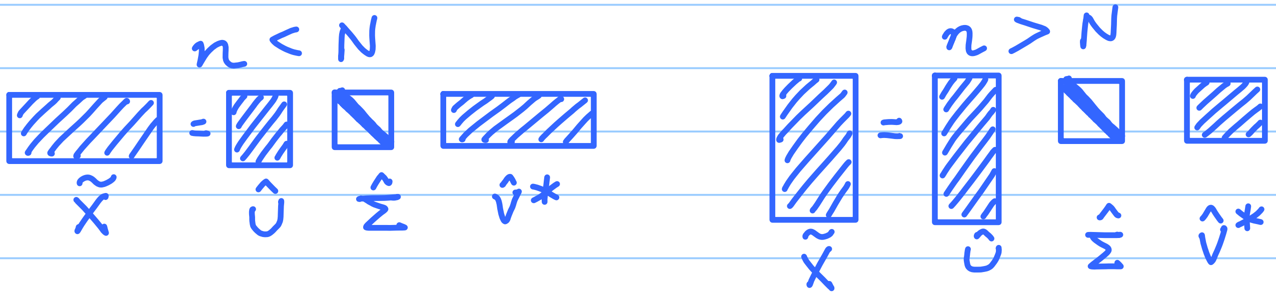
Remark : In either case ($n < N$ or $n > N$), you do not need to compute $\Gamma_{\tilde{X}}$. Moreover, you should use the reduced SVD instead of the full SVD for the purpose of KLB/PCA computation.

The reduced SVD of $\tilde{X} \in \mathbb{C}^{n\times N}$

$$\tilde{X} = \hat{U}\hat{\Sigma}\hat{V}^*$$

Let $p := \min(n, N-1) \geq r = \operatorname{rank}(\tilde{X})$.

Then $\hat{U} \in \mathbb{C}^{n\times p}$, $\hat{\Sigma} \in \mathbb{R}^{p\times p}$, $\hat{V} \in \mathbb{C}^{N\times p}$



In MATLAB, this is done by

```
>> [Û, Σ̂, V̂] = svd( X̃, 'econ');
```

Note also $\tilde{X}\hat{V} = \hat{U}\hat{\Sigma}\hat{V}^*\hat{V} = \hat{U}\hat{\Sigma}$

$$= [\sigma_1 u_1, \cdots \sigma_p u_p]$$

$$= [\tilde{X} v_1, \cdots, \tilde{X} v_p]$$

So, $u_j = \frac{1}{\sigma_j}\tilde{X} v_j$, $j = 1, \cdots, p = \min(n, N-1)$.
$= N-1$ if $n \gg N$.

In other words, each principal axis u_j is just a linear combination of the (centered) input vectors $\tilde{x}_1, \cdots, \tilde{x}_N$!

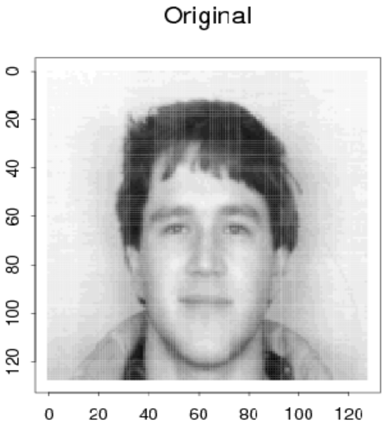
Example: The Rogues' Gallery Dataset

- Through the courtesy of Prof. Larry Sirovich
- A set of digitized photos of 143 faces each of which has 128×128 ixels i.e., $n = 128^2 = 16384$.
- These faces were of a specific group of people, i.e., Caucasian male students (and some faculty) at Brown Univ., without glasses, mustache, beard.
- Horizontal dilation has been applied s.t. the pupils are placed on two fixed common points.
- 143 faces were randomly divided into 72 and 71 faces for the training and test datasets, i.e., $N = 72$.
- KLB/PCA were computed on the training dataset.

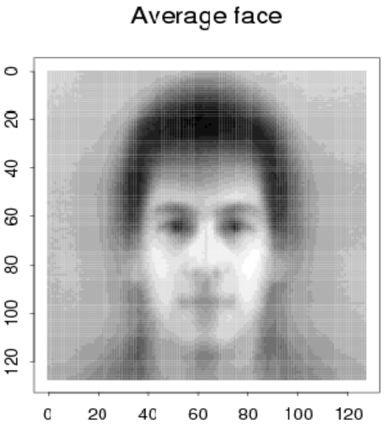
72 Faces !

$\mathbf{x}_1$ $\mathbf{x}_2$ . . .

$\mathbf{x}_{71}$ $\mathbf{x}_{72}$

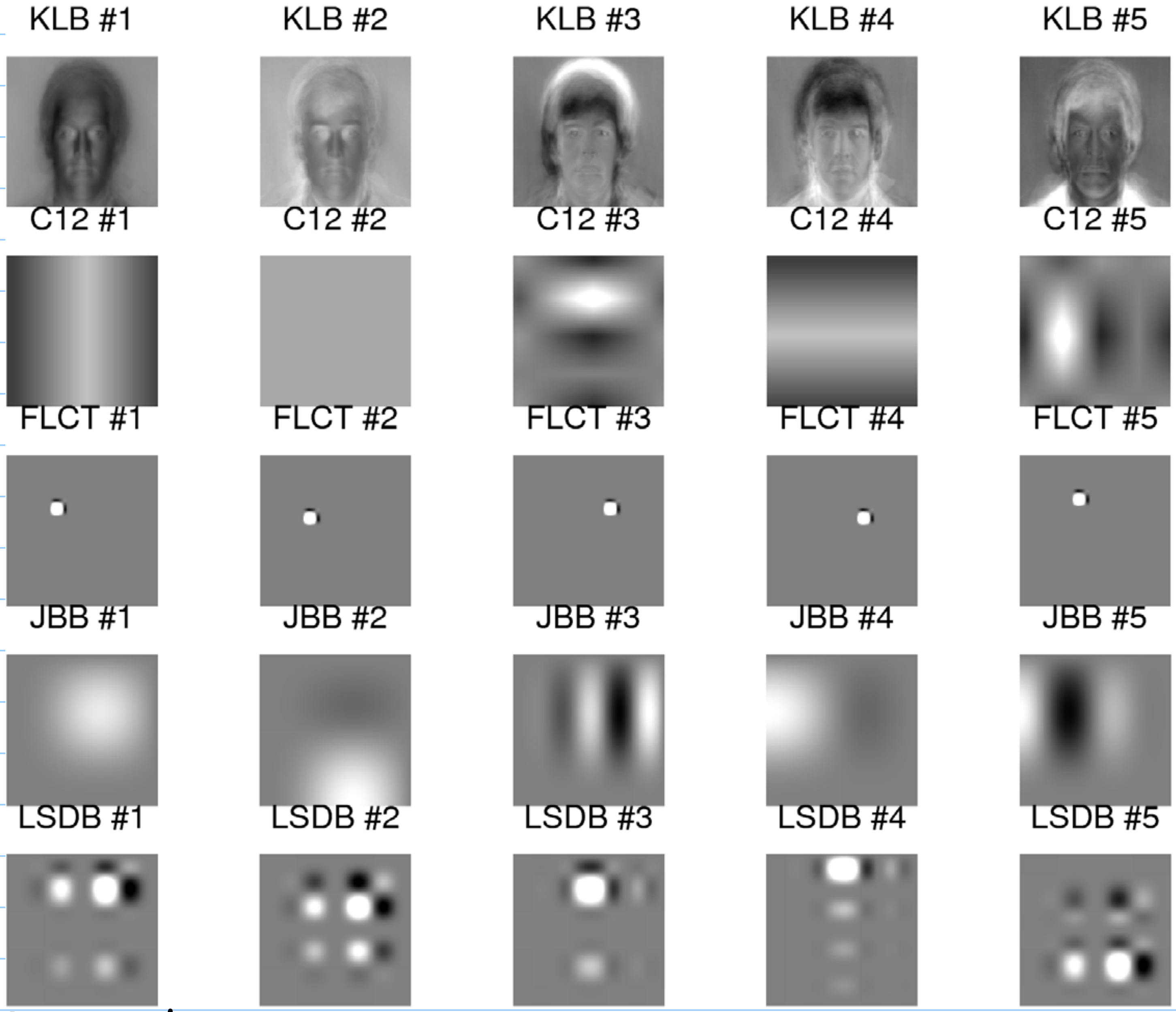


one of the test image



$\bar{\mathbf{x}}$

Comparison of Bases

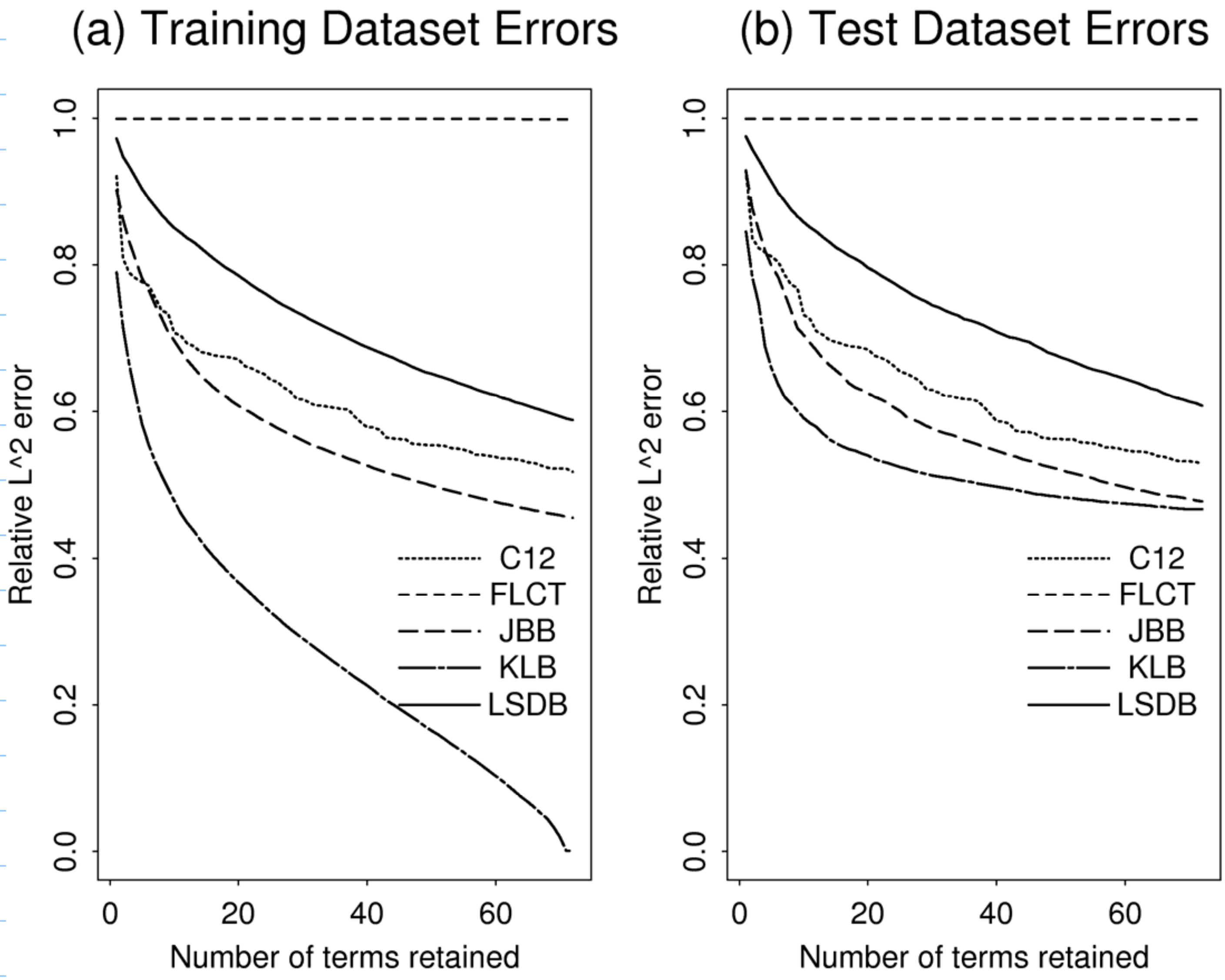


Remarks:

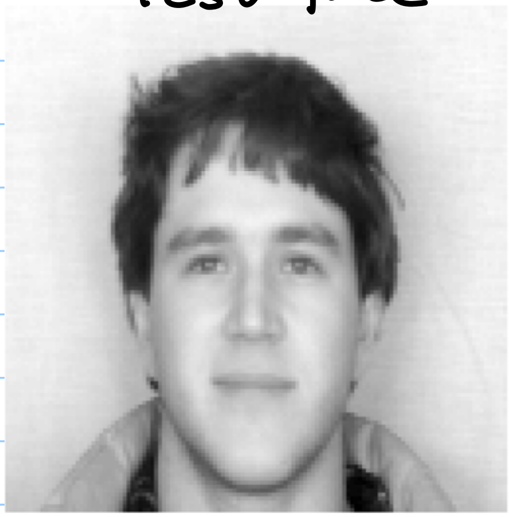
(1) I am only displaying the top 5 KLB vectors. There are totally 71 KLB vectors plus the mean vector $\overline{\mathbb{X}}$.

(2) As you can see these KLB vectors = lin. combi's of the 72 faces.

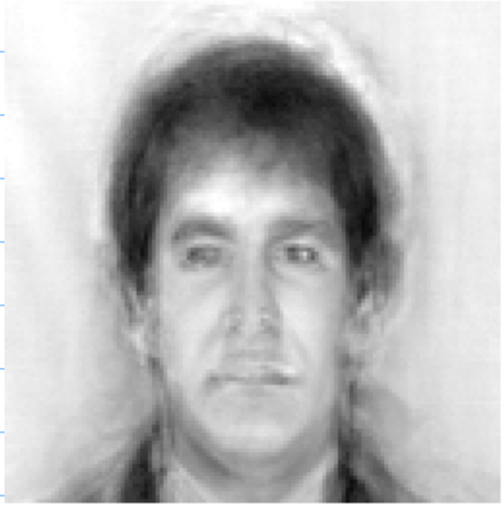
Approximation Errors



test face



71 term approx. + ave.



Remarks:

Note that for each training face, one can reconstruct it within machine precision using the full 71 KLB vectors and the average face $\bar{x}$.

However, for the test faces that were not used to generate the KLB, the reconstructions are not perfect.

Why? Basically, viewing these faces as the realizations of a stochastic process using only up to the 2nd order statistics (i.e., mean + covariance) and only using 72 realizations lead to serious limitation of the KLB applicability.

☆ Relationship between KLT and DCT

For simplicity, let's assume $E X_j = 0$, $j = 1:n$.
Suppose the underlying stochastic process is stationary in wide sense, i.e.,

$$\Gamma_{\mathbb{X}}[k, l] = \Gamma_{\mathbb{X}}[k+m, l+m], \quad \forall m \in \mathbb{Z}$$

(appropriate mod N needs here)

Furthermore, assume

$$\Gamma_{\mathbb{X}}[k, l] = \rho^{|k-l|} \qquad 0 < \rho < 1.$$

This is called the 1st order Markov model, i.e., X_{k+1} depends only on X_k (plus independent noise). This can be explained as follows.

Suppose $X_{k+1} = \rho X_k + Z_k$
where $\rho \in (0,1)$, Z_k : iid. $E Z_k = 0$
$\operatorname{var} Z_k = 1$.

Then

$$E X_k X_{k+1}^* = \rho E|X_k|^2 + \underbrace{E X_k Z_k}_{} = E X_k \underbrace{E Z_k}_{\overset{\shortparallel}{0}}$$

$$E X_k X_{k+2}^* = E X_k(\rho X_{k+1} + Z_{k+1})$$

$$= \rho E X_k X_{k+1} + \overset{0}{E X_k Z_{k+1}}$$

$$= \rho^2 E|X_k|^2$$

$$\vdots$$

$$E X_k X_{k+l}^* = \rho^l E|X_k|^2$$

Since we assumed the wide sense stationarity, $E|X_k|^2$ does not depend on k, i.e., we can assume

$E|X_k|^2 = \sigma^2 = \text{const.}$, and

$$\Gamma_{\mathbf{x}} = \sigma^2 \begin{bmatrix} 1 & \rho & \cdots & \rho^{n-1} \\ \rho & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \rho \\ \rho^{n-1} & \cdots & \rho & 1 \end{bmatrix} \Rightarrow \text{Toeplitz matrix!}$$

For further simplicity, let's assume $\sigma^2=1$.

One can show that

The eigenvalues & eigenvectors of this Toeplitz matrix are:

$$\begin{cases} \lambda_k = \dfrac{1-\rho^2}{1-2\rho\cos\omega_k+\rho^2}, & k=0,1,\cdots,n-1. \\ w_k[l] = \sqrt{\dfrac{2}{n+\lambda_k}}\,\sin\left[\omega_k\left(l-\left(\frac{n-1}{2}\right)\right)+(k+1)\frac{\pi}{2}\right] & l=0,1,\cdots,n-1. \end{cases}$$

where ω_k is a solution of the following secular equation:

$$\tan(n\omega_k) = -\frac{(1-\rho^2)\sin\omega_k}{(1+\rho^2)\cos\omega_k-2\rho}$$

Now consider the case when $\rho \uparrow 1$.

Then $\tan n\omega_k = 0 \iff \omega_k = \frac{k\pi}{n}$, $k \neq 0$

For $k=0$, we use the small angle perturbation: $\tan\alpha \approx \alpha$, $\sin\alpha \approx \alpha$, $\cos\alpha \approx 1-\frac{\alpha^2}{2}$

Using these, we get

$$n\,\cancel{\omega_0} = -\frac{(1-\rho^2)\cancel{\omega_0}}{(1+\rho^2)(1-\omega_0^2/2)-2\rho}$$

$$\Longleftrightarrow \omega_0^2 = \frac{2}{1+\rho^2}\cdot\frac{1-\rho^2}{n} + \frac{2(1-\rho)^2}{1+\rho^2}$$

$$\approx \frac{1}{n}(1-\rho^2) \quad \text{as } \rho \uparrow 1.$$

So, one can say $\omega_0 \to 0$ as $\rho \uparrow 1$.
after all, $\omega_k = k\pi/n$, $k=0,1,\cdots,n-1$.

Now, $$\mathbf{w}_k[l] = \sqrt{\frac{2}{n+\lambda_k}}\sin\left[\frac{k\pi}{n}\left(l-\left(\frac{n-1}{2}\right)\right)+(k+1)\frac{\pi}{2}\right]$$

$$= \sqrt{\frac{2}{n+\lambda_k}}\sin\left[\frac{\pi k}{n}\left(l+\frac{1}{2}\right)+\frac{\pi}{2}\right]$$

$$= \sqrt{\frac{2}{n+\lambda_k}}\,\underline{\cos\left[\frac{\pi k}{n}\left(l+\frac{1}{2}\right)\right]}$$

How about λ_k as $\rho \uparrow 1$?

For $k \neq 0$, $$\lambda_k = \frac{1-\rho^2}{1-2\rho\cos\omega_k+\rho^2} \to 0 \quad \text{as } \rho \uparrow 1$$

For $k=0$, $$\lambda_0 \approx \frac{1-\rho^2}{1-2\rho(1-\omega_0^2/2)+\rho^2}$$

$$= \frac{1+\rho}{1-\rho+\rho(1+\rho)/n}$$

$$\underline{\to n \quad \text{as } \rho \uparrow 1.}$$

So, $$\begin{cases} \mathbf{w}_0[l] = \dfrac{1}{\sqrt{n}} \\ \mathbf{w}_k[l] = \sqrt{\dfrac{2}{n}}\cos\left[\dfrac{\pi k(l+\frac{1}{2})}{n}\right] \end{cases}$$ DCT-II !!