

Eigenvectors in Cross Data Matrix Method

Shao-Hsuan Wang

Joint work with Dr. Su-Yun Huang and Dr. Ting-Li Chen

February 1, 2019



- High-dimension, low-sample -size (HDLSS) data occurs in many modern science fields such as genetic microarrays, medical imaging, text recognition, finance, chemometrics, and so on.
- Principal Component Analysis (PCA) is an important tool for dimension reduction especially when the dimension is very high.



- $d \rightarrow \infty$: see Johnstone (2001), Baik (2005), and Pual (2007) for Gaussian assumptions.
- $d/n \rightarrow c > 0$: see Baik and Silverstein (2006) for non-Gaussian assumptions.
- $d/n \rightarrow 0$: see Johnstone and Lu (2009).
- $d \rightarrow \infty$ and n is fixed: see Hall et al. (2005) and Ahn et al. (2007).



- Yata and Aoshima (2009): more general settings without assuming either the normality or ρ -mixing condition





ELSEVIER

Journal of Multivariate Analysis

Volume 101, Issue 9, October 2010, Pages 2060-2077

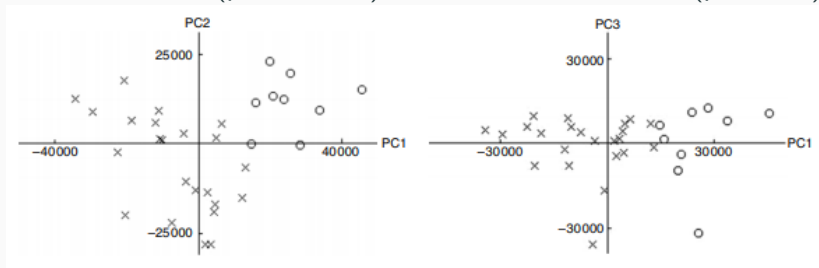


Effective PCA for high-dimension, low-sample-size data with singular value decomposition of cross data matrix

Kazuyoshi Yata ^a, Makoto Aoshima ^b  

Example

The dataset contains 34 patients with 12600 genes. There are 9 Normal Prostate (plotted as o) and 25 Prostate Tumors (plotted x)

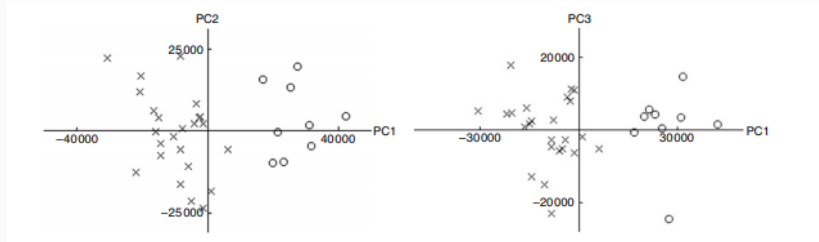


(PCA)



Example

The dataset contains 34 patients with 12600 genes. There are 9 Normal Prostate (plotted as o) and 25 Prostate Tumors (plotted x)



(cross-PCA)

- Yata and Aoshima (2010)'s general setting
- PCA vs cross-PCA
 1. Consistency for eigenvectors (Yata and Aoshima)
 2. Asymptotic normality for eigenvectors (Our work)
- Simulation Results

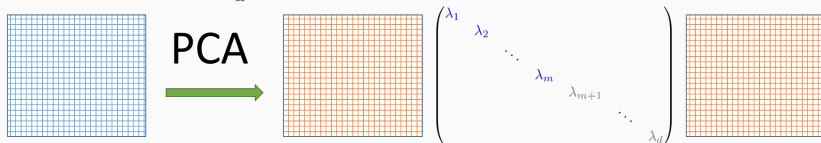


Yata and Aoshima (2010)'s general setting

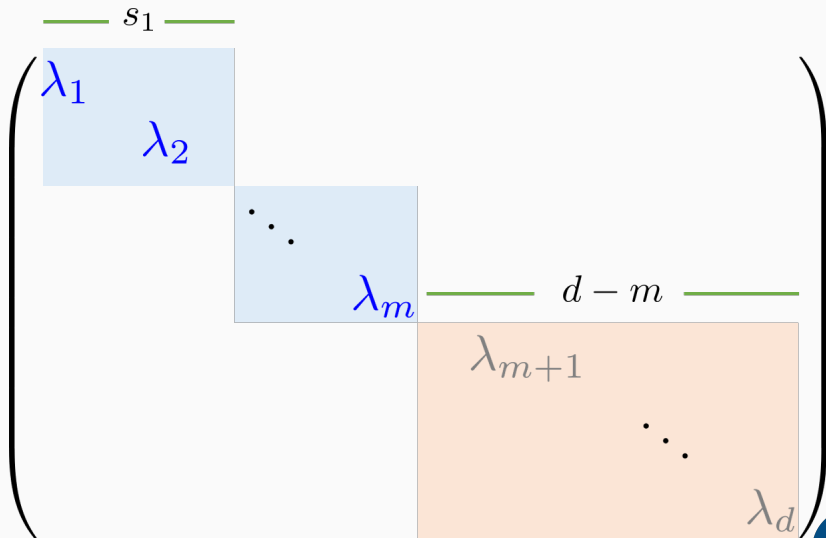
$$\lambda_i = a_i d^{\alpha_i} \ (i = 1, \dots, m) \text{ and } \lambda_j = c_j \ (j = m + 1, \dots, d).$$

Here $a_i > 0$, $c_j \geq 0$ and $\alpha_1 > \alpha_2 > \dots > \alpha_m$ preserving

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d.$$



Yata and Aoshima (2010)'s general setting



$$s_1 + \cdots + s_u + \cdots s_J = m$$



Some interesting facts

- PCA:

$\mathbf{X}\mathbf{X}^\top$ and its dual matrix $\mathbf{X}^\top\mathbf{X}$

- (a) $d \times d$ vs $n \times n$ (In general, one of them needs to be small).
- (b) Share the same eigenvalues in the sample covariance matrix.
- (c) Not share the same eigenvalues in the population covariance matrix.

- cross-PCA:

$\mathbf{X}_{(1)}^\top\mathbf{X}_{(2)}$ and $\mathbf{X}_{(2)}^\top\mathbf{X}_{(1)}$ (cross data matrix)

- (a) Share the same eigenvalues in the sample covariance matrix.
- (b) Not share the same eigenvalues in the population covariance matrix.



Theorem (PCA) Suppose that

- (i) $d \rightarrow \infty$ and $n \rightarrow \infty$ for i such that $\alpha_i > 1$.
- (ii) $d \rightarrow \infty$ and $d^{2-2\alpha_i}/n \rightarrow 0$ for i such that $\alpha_i \in (0, 1]$.

For $1 = 1, \dots, m$, as $d \rightarrow \infty$. Then

- (a) $\text{Angle}(\hat{\mathbf{h}}_i, \mathbf{h}_i) \rightarrow 0$ in probability.
- (b) $\text{Angle}(\hat{\mathbf{h}}_i, \mathbf{h}_k) \rightarrow \frac{\pi}{2}$, $k = m+1, \dots, d$ in probability.

Theorem (cross-PCA) Suppose that

- (i) $d \rightarrow \infty$ and $n \rightarrow \infty$ for i such that $\alpha_i > 1$.
- (ii) $d \rightarrow \infty$ and $d^{1-\alpha_i}/n \rightarrow 0$ for i such that $\alpha_i \in (1/2, 1]$.
- (iii) $d \rightarrow \infty$ and $d^{2-2\alpha_i}/n \rightarrow 0$ for i such that $\alpha_i \in (0, 1/2]$.

For $1 = 1, \dots, m$, as $d \rightarrow \infty$. Then

- (a) $\text{Angle}(\tilde{\mathbf{h}}_i^*, \mathbf{h}_i) \rightarrow 0$ in probability.
- (b) $\text{Angle}(\tilde{\mathbf{h}}_i^*, \mathbf{h}_k) \rightarrow \frac{\pi}{2}$, $k = m+1, \dots, d$ in probability.



Our work (PCA)

Theorem (PCA) Suppose that Yata and Aoshima's PCA conditions hold. Assume that the first m population eigenvalues are distinct. Consider the j th eigenvector, where $s_{u-1} < j \leq s_u$. Then, we have (a)

$$\sqrt{n} \text{vec} \left[\left(\hat{\mathbf{h}}_{j(1)} - \mathbf{h}_j, \hat{\mathbf{h}}_{j(2)} - \mathbf{h}_j \right)^\top \mathbf{H}_{[1:m]} \right] \Rightarrow N \left(\mathbf{0}, \boldsymbol{\psi}^{[j]} \right),$$

where $\boldsymbol{\psi}^{[j]}$ is a block matrix consisting of $m \times m$ blocks, and each block is of size 2×2 . Precisely, $\boldsymbol{\psi}^{[j]}$ takes the following form: its (k, k') th block is given by

$$\boldsymbol{\psi}_{kk}^{[j]} = \begin{cases} \frac{a_k a_j}{(a_k - a_j)^2} \text{E}[z_{11(1)}^2 z_{21(1)}^2], & k \neq j \\ 0, & k = j \end{cases}$$

and its (k, k') th block, where $s_{u-1} < k, k' \leq s_u$, is given by

$$\boldsymbol{\psi}_{kk'}^{[j]} = \frac{a_k a_{k'} a_j^2}{(a_k - a_j)(a_{k'} - a_j)} \text{E}[z_{11(1)} z_{21(1)} z_{31(1)}^2],$$

and all other blocks are zero matrices, i.e., $\boldsymbol{\psi}_{kk'}^{[j]} = \mathbf{0}_{2 \times 2}$ for k, k' not being in the same eigen-groups.



Our work (PCA)

(b)

$$\left\| \left(\hat{\mathbf{h}}_{j(1)} - \mathbf{h}_j, \hat{\mathbf{h}}_{j(2)} - \mathbf{h}_j \right)^\top \mathbf{H}_{\text{tail}} \right\|_2 = o_p \left(n^{-1/4} \right).$$

Corollary (full-PCA)

Assume that the first s_1 population eigenvalues are distinct. Consider the j th eigenvector, $1 \leq j \leq s_1$. Then, we have, for $1 \leq k \leq s_1$

$$\sqrt{2n} \mathbf{h}_k^\top (\hat{\mathbf{h}}_j - \mathbf{h}_j) \Rightarrow N \left(0, \frac{a_k a_j}{(a_k - a_j)^2} \mathbb{E}[z_{11(1)}^2 z_{21(1)}^2] \right), \quad k \neq j,$$

$$\sqrt{2n} \mathbf{h}_j^\top (\hat{\mathbf{h}}_j - \mathbf{h}_j) = o_p(1).$$



Our work (cross-PCA)

Theorem (cross-PCA) Suppose that Yata and Aoshima's cross-PCA conditions hold. Assume that the first m population eigenvalues are distinct. Consider the j th eigenvector, where $s_{u-1} < j \leq s_u$. Then, we have (a)

$$\sqrt{n} \text{vec} \left[\left(\tilde{\mathbf{h}}_{j(1)} - \mathbf{h}_j, \tilde{\mathbf{h}}_{j(2)} - \mathbf{h}_j \right)^\top \mathbf{H}_{[1:m]} \right] \Rightarrow N \left(\mathbf{0}, \mathbf{M}^{[j]} \right),$$

where $\mathbf{M}^{[j]}$ is a block matrix consisting of $m \times m$ blocks, and each block is of size 2×2 . Precisely, $\mathbf{M}^{[j]}$ takes the following form: its $(k, k')^{\text{th}}$ block is given by

$$\mathbf{M}_{kk'}^{[j]} = \begin{cases} \frac{a_k a_j}{(a_k - a_j)^2} \mathbb{E}[z_{11(1)}^2 z_{21(1)}^2] \begin{pmatrix} \frac{a_k^2 + a_j^2}{(a_k + a_j)^2} & \frac{2a_k a_j}{(a_k + a_j)^2} \\ \frac{2a_k a_j}{(a_k + a_j)^2} & \frac{a_k^2 + a_j^2}{(a_k + a_j)^2} \end{pmatrix}, & k \neq j \\ 0, & k = j \end{cases}$$

and its $(k, k')^{\text{th}}$ block, where $s_{u-1} < k, k' \leq s_u$, is given by

$$\mathbf{M}_{kk'}^{[j]} = \begin{cases} \frac{a_k a_{k'} a_j^2}{(a_k - a_j)(a_{k'} - a_j)} \mathbb{E}[z_{11(1)} z_{21(1)} z_{31(1)}^2] \begin{pmatrix} \frac{a_j^2 + a_j a_k}{(a_j + a_k)(a_j + a_{k'})} & \frac{a_j(a_k + a_{k'})}{(a_j + a_k)(a_j + a_{k'})} \\ \frac{a_j(a_k + a_{k'})}{(a_j + a_k)(a_j + a_{k'})} & \frac{a_j^2 + a_j a_{k'}}{(a_j + a_k)(a_j + a_{k'})} \end{pmatrix}, & k, k' \neq j \\ 0 & k = j \text{ or } k' = j \end{cases}$$

and all other blocks are zero matrices, i.e., $\mathbf{M}_{kk'}^{[j]} = \mathbf{0}_{2 \times 2}$ for k, k' not being in the same eigen-groups.



Our work(cross-PCA)

(b)

$$\left\| \left(\tilde{\mathbf{h}}_{j(1)} - \mathbf{h}_j, \tilde{\mathbf{h}}_{j(2)} - \mathbf{h}_j \right)^\top \mathbf{H}_{\text{tail}} \right\|_2 = o_p \left(n^{-1/4} \right).$$

Corollary (cross-PCA)

Let $\tilde{\mathbf{h}}_j = \{ \tilde{\mathbf{h}}_{j(1)} + \text{sign}(\tilde{\mathbf{h}}_{j(1)}^\top \tilde{\mathbf{h}}_{j(2)}) \tilde{\mathbf{h}}_{j(2)} \}$ and $\tilde{\mathbf{h}}_j^* = \tilde{\mathbf{h}}_j / \|\tilde{\mathbf{h}}_j\|$. Assume that the first s_1 population eigenvalues are distinct. Consider the j th eigenvector, $1 \leq j \leq s_1$. Then, we have, for $1 \leq k \leq s_1$

$$\sqrt{2n} \mathbf{h}_k^\top (\tilde{\mathbf{h}}_j^* - \mathbf{h}_j) \Rightarrow N \left(0, \frac{a_k a_j}{(a_k - a_j)^2} \mathbb{E}[z_{11(1)}^2 z_{21(1)}^2] \right), \quad k \neq j,$$

$$\sqrt{2n} \mathbf{h}_j^\top (\tilde{\mathbf{h}}_j^* - \mathbf{h}_j) = o_p(1).$$



Asymptotics results

1. Based on the inequality $1 \leq 2(a_j^2 + a_k^2)/(a_j + a_k)^2 \leq 2$, for $k, j = 1, \dots, s_1$

$$\lim_{n \rightarrow \infty} \text{var}(\mathbf{h}_k^\top \hat{\mathbf{h}}_j) \leq \lim_{n \rightarrow \infty} \text{var}(\mathbf{h}_k^\top \tilde{\mathbf{h}}_{j(i)}) \leq \lim_{n \rightarrow \infty} \text{var}(\mathbf{h}_k^\top \hat{\mathbf{h}}_{j(i)}).$$

2. Let $\tilde{\mathbf{h}}_j^w = \tilde{\mathbf{h}}_j / \sqrt{2}$. Then for $k, j = 1, \dots, s_1$

$$\lim_{n \rightarrow \infty} \text{var}(\sqrt{2n} \mathbf{h}_k^\top \hat{\mathbf{h}}_j) = \lim_{n \rightarrow \infty} \text{var}(\sqrt{n} \mathbf{h}_k^\top \tilde{\mathbf{h}}_j^w) = \lim_{n \rightarrow \infty} \text{var}(\sqrt{2n} \mathbf{h}_k^\top \tilde{\mathbf{h}}_j^*).$$

3. Define $\text{ave}_{\text{tail}} \mathbf{h}_\ell^\top \tilde{\mathbf{h}}_{j(i)} = \sum_{\ell=m+1}^d \mathbf{h}_\ell^\top \tilde{\mathbf{h}}_{j(i)} / (d - m + 1)$. Then

$$\text{ave}_{\text{tail}} \mathbf{h}_\ell^\top \tilde{\mathbf{h}}_{j(i)} = o_p(n^{-1/2}).$$

Further, $\text{ave}_{\text{tail}} \mathbf{h}_\ell^\top \tilde{\mathbf{h}}_{j(i)} / \mathbf{h}_k^\top \tilde{\mathbf{h}}_{j(i)} = o_p(1)$, $k = 1, \dots, m$.



cross-PCA: A sketch of proof

(S1) Starting with

$$\mathbf{S}_{D(1)} \mathbf{S}_{D(1)}^\top \tilde{\mathbf{u}}_{j(1)} = \tilde{\lambda}_j^2 \tilde{\mathbf{u}}_{j(1)}, \quad j = 1, \dots, n. \quad (1)$$

Let $\mathbf{W} = n^{-2} \mathbf{X}_{(1)} \mathbf{X}_{(1)}^\top \mathbf{X}_{(2)} \mathbf{X}_{(2)}^\top$. Thus, multiplying both sides of (1) by $\mathbf{X}_{(1)}$,

$$\mathbf{W}(\mathbf{X}_{(1)} \tilde{\mathbf{u}}_{j(1)}) = \tilde{\lambda}_j^2 (\mathbf{X}_{(1)} \tilde{\mathbf{u}}_{j(1)}) \text{ and } \mathbf{W} \tilde{\mathbf{h}}_{j(1)} = \tilde{\lambda}_j^2 \tilde{\mathbf{h}}_{j(1)}, \quad j = 1, \dots, n$$

Note that $\tilde{\mathbf{h}}_{j(1)} = (n \tilde{\lambda}_j)^{-1/2} \mathbf{X}_{(1)} \tilde{\mathbf{u}}_{j(1)}$, $j = 1, \dots, n$. Based on the independence of $\mathbf{X}_{(1)}$ and $\mathbf{X}_{(2)}$, $\mathbf{E}\mathbf{W} = \mathbf{\Sigma}^2 = \mathbf{H} \mathbf{\Lambda}^2 \mathbf{H}^\top$. Let $\mathbf{\Sigma}^* = \mathbf{\Sigma}^2$ and $\mathbf{\Lambda}^* = \mathbf{\Lambda}^2$. Let $\lambda_j^* = \lambda_j^2$ and $\tilde{\lambda}_j^* = \tilde{\lambda}_j^2$. Thus we have $\mathbf{\Sigma}^* \mathbf{h}_j = \lambda_j^* \mathbf{h}_j$.

Proposition (perturbation method). For fixed m ,

$$(\mathbf{\Sigma}_{[m]}^* + \epsilon \dot{\mathbf{\Sigma}}_{[m]}^*)(\mathbf{h}_{j[m]} + \epsilon \dot{\mathbf{h}}_{j[m]}) = (\lambda_{j[m]}^* + \epsilon \dot{\lambda}_{j[m]}^*)(\mathbf{h}_{j[m]} + \epsilon \dot{\mathbf{h}}_{j[m]}),$$

implying $\dot{\mathbf{h}}_{j[m]} = (\lambda_{j[m]}^* \mathbf{I}_m - \mathbf{\Sigma}_{[m]}^*)^+ \dot{\mathbf{\Sigma}}_{[m]}^* \mathbf{h}_{j[m]}$, $j = 1, \dots, n$. Here, $\epsilon \dot{\mathbf{\Sigma}}_{[m]}^* = \tilde{\mathbf{\Sigma}}_{[m]}^* - \mathbf{\Sigma}_{[m]}^*$.

$\epsilon \dot{\mathbf{h}}_{j[m]} = \tilde{\mathbf{h}}_{j(i)[m]} - \mathbf{h}_{j[m]}$, and $\epsilon \dot{\lambda}_{j[m]}^* = \tilde{\lambda}_{j[m]}^* - \lambda_{j[m]}^*$.



cross-PCA: A sketch of proof

(S2) By the consistency results from Yata and Aoshima (2010), the perturbation method allows us to consider the j th eigenvector and the respective matrix $H_{1 \setminus j}$, $1 \leq j \leq s_1$. It implies that

$$\begin{aligned}
 H_{1 \setminus j}^\top \dot{h}_j &= H_{1 \setminus j}^\top (\lambda_j^* I_d - \Sigma^*)^+ \dot{\Sigma}^* h_j \\
 &= \left(\frac{1}{\lambda_j^* - \lambda_k^*} h_k^\top \dot{\Sigma}^* h_j \right)_{k \in \{1, \dots, s_1\} \setminus j} = \left(\frac{1}{\lambda_j^* - \lambda_k^*} (h_j^\top \otimes h_k^\top) \text{vec} \dot{\Sigma}^* \right)_{k \in \{1, \dots, s_1\} \setminus j}, \\
 h_j^\top \dot{h}_j &= 0.
 \end{aligned} \tag{2}$$

As for the right hand side of (2), we consider the perturbation of its component with the index k :

$$\begin{aligned}
 \frac{1}{\lambda_j^* - \lambda_k^*} (h_j^\top \otimes h_k^\top) (\text{vec} W - \text{vec} \Sigma^*) &= \frac{1}{\lambda_j^* - \lambda_k^*} (h_j^\top \otimes h_k^\top) \{ (I_d \otimes S_{(1)}) \text{vec} S_{(2)} - (I_d \otimes \Sigma) \text{vec} \Sigma \} \\
 &= \frac{1}{\lambda_j^* - \lambda_k^*} (h_j^\top \otimes h_k^\top) \{ I_d \otimes (S_{(1)} - \Sigma) \} \text{vec} S_{(2)} \\
 &\quad + \frac{1}{\lambda_j^* - \lambda_k^*} (h_j^\top \otimes h_k^\top) (I_d \otimes \Sigma) (\text{vec} S_{(2)} - \text{vec} \Sigma),
 \end{aligned} \tag{3}$$

where $S_{(1)} = n^{-1} X_{(1)} X_{(1)}^\top$ and $S_{(2)} = n^{-1} X_{(2)} X_{(2)}^\top$.



cross-PCA: A sketch of proof

(S3)

$$\begin{aligned} & \frac{\sqrt{n}}{\lambda_j^* - \lambda_k^*} (\mathbf{h}_j^\top \otimes \mathbf{h}_k^\top) (\text{vec} \mathbf{W} - \text{vec} \mathbf{\Sigma}^*) \\ &= \frac{\sqrt{\lambda_j \lambda_k}}{\lambda_j - \lambda_k} \frac{\sqrt{n}}{n} \sum_{s=1}^n \left\{ \frac{\lambda_j}{\lambda_j + \lambda_k} z_{ks(1)} z_{js(1)} + \frac{\lambda_k}{\lambda_j + \lambda_k} z_{ks(2)} z_{js(2)} \right\} + o_p(1). \end{aligned}$$

$$\begin{aligned} & \sqrt{n} \mathbf{H}_{1 \setminus j}^\top (\tilde{\mathbf{h}}_{j(1)} - \mathbf{h}_j) \\ &= \frac{\sqrt{n}}{n} \sum_{s=1}^n \left(\frac{\sqrt{a_j a_k}}{a_j - a_k} \left\{ \frac{a_j}{a_j + a_k} z_{(1)ks} z_{(1)js} + \frac{a_k}{a_j + a_k} z_{(2)ks} z_{(2)js} \right\} \right)_{k \in \{1, \dots, s_1\} \setminus j} (1 + o_p(1)) \\ &+ o_p(1) \end{aligned}$$

and

$$\sqrt{n} \mathbf{h}_j^\top \tilde{\mathbf{h}}_{j(1)} = o_p(1).$$



Simulation Results



- Sample size $n = 100$
- `data_set = 'truncated-t'`
- $d = 10^5$
- The first four eigenvalues $16d^{2/3}, 4d^{2/3}, d^{1/3}, d^{1/3}$ with $s_1 = 2$.
- Run 1000 times

	Half-PCA		Full-PCA		Cross-PCA	
	$\sqrt{n}\mathbf{h}_1^\top \hat{\mathbf{h}}_{2(1)}$	$\sqrt{n}\mathbf{h}_2^\top \hat{\mathbf{h}}_{1(1)}$	$\sqrt{2n}\mathbf{h}_1^\top \hat{\mathbf{h}}_2$	$\sqrt{2n}\mathbf{h}_2^\top \hat{\mathbf{h}}_1$	$\sqrt{2n}\mathbf{h}_1^\top \hat{\mathbf{h}}_2^*$	$\sqrt{2n}\mathbf{h}_2^\top \hat{\mathbf{h}}_1^*$
<i>mean</i>	0.015	-0.069	0.025	-0.007	0.013	0.004
<i>var</i>	1.144	1.140	0.670	0.671	0.600	0.606
	Half-PCA		Full-PCA		Cross-PCA	
	$\sqrt{n}(\mathbf{h}_1^\top \hat{\mathbf{h}}_{1(1)} - 1)$	$\sqrt{n}(\mathbf{h}_2^\top \hat{\mathbf{h}}_{2(1)} - 1)$	$\sqrt{2n}(\mathbf{h}_1^\top \hat{\mathbf{h}}_1 - 1)$	$\sqrt{2n}(\mathbf{h}_2^\top \hat{\mathbf{h}}_2 - 1)$	$\sqrt{2n}(\mathbf{h}_1^\top \hat{\mathbf{h}}_1^* - 1)$	$\sqrt{2n}(\mathbf{h}_2^\top \hat{\mathbf{h}}_2^* - 1)$
<i>mean</i>	-0.090	-0.090	-0.036	-0.037	-0.031	-0.031
<i>var</i>	0.2205	0.2204	0.049	0.049	0.008	0.007

