Population Principal Components

- **Result 8.1:** Let Σ be the covariance matrix of $X' = (X_1, X_2, \cdots, X_p)$

Let Σ have eigen-pairs $(\lambda_1, e_1), (\lambda_2, e_2), \cdots, (\lambda_p, e_p)$ where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p > 0$

Then the i-th principal component is given by $Y_i = e_i' X = e_{i1} X_1 + e_{i2} X_2 + \cdots + e_{ip} X_p$

With these, $Var(Y_i) = e_i' \Sigma e_i = \lambda_i$, $cov(Y_i, Y_k) = e_i' \Sigma e_k = 0$

- **Result 8.2:** Let $X' = (X_1, X_2, \cdots, X_p)$ have covariance matrix Σ, with eigen-pairs $(\lambda_1, e_1), (\lambda_2, e_2), \cdots, (\lambda_p, e_p)$ where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$. Let $Y_1 = e_1' X$, $Y_2 = e_2' X$, $\cdots$, $Y_p = e_p' X$

Then $\sigma_{11} + \sigma_{22} + \cdots + \sigma_{nn} = \sum_{i=1}^{p} Var(X_i) = \lambda_1 + \lambda_2 + \cdots + \lambda_p = \sum_{i=1}^{p} Var(Y_i)$

proof: $\sigma_{11} + \sigma_{12} + \cdots + \sigma_{nn} = tr(\Sigma) = tr(P \Lambda P') = tr(\Lambda) = \lambda_1 + \lambda_2 + \cdots + \lambda_p$

- **Result 8.3:** If $Y_1 = e_1' X$, $Y_2 = e_2' X$ $\cdots$ $Y_p = e_p' X$ are principal components

Then $\rho(Y_i, X_k) = \frac{e_{ik} \sqrt{\lambda_i}}{\sqrt{\sigma_{kk}}}$ are coefficients between the components Y_i and X_k

proof: $\rho(Y_i, X_k) = \frac{cov(Y_i, X_k)}{\sqrt{Var(Y_i)} \sqrt{Var(X_k)}} = \frac{\lambda_i e_{ik}}{\sqrt{\lambda_i} \sqrt{\sigma_{kk}}} = \frac{e_{ik} \sqrt{\lambda_i}}{\sqrt{\sigma_{kk}}}$

Remark: Coefficients and correlations are both important.

Principal Components from Standardized Variables

- Standardized variable: $Z_1 = \frac{X_1 - \mu_1}{\sqrt{\sigma_{11}}}, Z_2 = \frac{X_2 - \mu_2}{\sqrt{\sigma_{22}}}, \cdots, Z_p = \frac{X_p - \mu_p}{\sqrt{\sigma_{pp}}}$

  or

  (Matrix Rotation): $Z = (V^{1/2})^{-1}(X-\mu)$ where $V = \mathrm{diag}\{\sigma_{11}, \sigma_{22}, \cdots, \sigma_{nn}\}$

  And $\mathrm{Cov}(Z) = V^{-1/2}\Sigma V^{-1/2} = \rho$ is the correlation matrix of X

- Result 8.4 The ith principal component of standardized variables $Z' = (Z_1, Z_2, \cdots Z_p)$ with $\mathrm{Cov}(Z) = \rho$ is given by $Y_i = e_i' V^{-1/2}(X-\mu)$.

  Moreover, $\sum_{i=1}^{p} \mathrm{Var}(Y_i) = \sum_{i=1}^{p} \mathrm{Var}(Z_i) = p$ and $\rho(Y_i, Z_k) = e_{ik}\sqrt{\lambda_i}$

- Remark: Proportion of variance due to k-th principal component $= \frac{\lambda_k}{p}$

  Principal Components of Σ and ρ are different.

Special cases: $\rho = \begin{pmatrix} 1 & \rho & \cdots & \rho \\ \rho & 1 & \cdots & \rho \\ \vdots & \vdots & & \vdots \\ \rho & \rho & \cdots & 1 \end{pmatrix}$, then $\lambda_1 = 1 + (p-1)\rho$, $e_1' = (\frac{1}{\sqrt{p}}, \frac{1}{\sqrt{p}}, \cdots, \frac{1}{\sqrt{p}})$

$\lambda_2, \cdots, \lambda_p = 1 - \rho$, $e_2', \cdots, e_p' = (\frac{1}{\sqrt{(i-1)i}}, \cdots, \frac{-(i-1)}{\sqrt{(i-1)i}}, 0 \cdots)$

explained proportion $= \frac{\lambda_1}{p} = \rho + \frac{1-\rho}{p}$

Principal Components for Samples

- Sample Covariance: $S=\frac{1}{n-1}\sum_{i=1}^{n}(X_i-\bar{X})(X_i-\bar{X})^T$

If S has eigen-pairs $(\hat{\lambda}_1,\hat{e}_1),(\hat{\lambda}_2,\hat{e}_2),\cdots,(\hat{\lambda}_p,\hat{e}_p)$, then the i-th component will be given by $\hat{y}_i=\hat{e}_i'x=\hat{e}_{i1}x_1+\hat{e}_{i2}x_2+\cdots+\hat{e}_{ip}x_p$

If $\hat{\lambda}_1>\hat{\lambda}_2>\cdots>\hat{\lambda}_p$, sample variance $(\hat{y}_k)=\hat{\lambda}_k$

sample covariance $(\hat{y}_i,\hat{y}_k)=0$

Total sample variance $=\sum_{i=1}^{p}s_{ii}=\hat{\lambda}_1+\hat{\lambda}_2+\cdots+\hat{\lambda}_p$

Correlation $\hat{r}(\hat{y}_i,x_k)=\frac{\hat{e}_{ik}\sqrt{\hat{\lambda}_i}}{\sqrt{s_{kk}}}$

- Remark: If $\hat{y}_i=\hat{e}_i'(x_i-\bar{x})$ is centralized, then $\hat{y}_i$ is centralized at 0.

$$\overline{\hat{y}_i}=\frac{1}{n}\sum_{i=1}^{n}\hat{e}_i'(x_j-\bar{x})=\frac{1}{n}\hat{e}_i'\left(\sum_{j=1}^{n}(x_j-\bar{x})\right)=\frac{1}{n}\hat{e}_i'\cdot 0=0$$

sample principal components are not either invariant with respect to changes in scale.