On the identification of common principal components

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What are common principal components (CPCs)?

How can covariance structures of two groups differ?

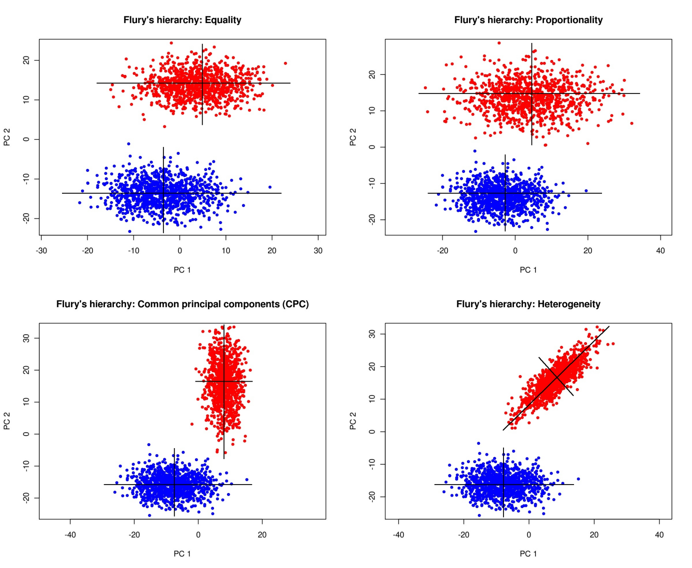
Univariate:

- Homoscedastic or heteroscedastic (nothing in between)

Multivariate case:

- Flury's hierarchy (1988):
  1. Equality $\mathbf{\Sigma}_1 = \mathbf{\Sigma}_2$
  2. Proportionality $\mathbf{\Sigma}_1 = \rho\mathbf{\Sigma}_2$
  3. Common principal components
  4. Partial common principal components
  5. Heterogeneity

What are CPCs?



What are CPCs?

Principal component analysis (PCA):

$$\mathbf{\Sigma} = \boldsymbol{B}\mathbf{\Lambda}\boldsymbol{B}'$$

Common principal components (CPC):

$$\mathbf{\Sigma}_1 = \boldsymbol{B}\mathbf{\Lambda}_1\boldsymbol{B}'$$

$$\mathbf{\Sigma}_2 = \boldsymbol{B}\mathbf{\Lambda}_2\boldsymbol{B}'$$

Partial common principal components (CPC(q)):

$$\begin{array}{lcl} \mathbf{\Sigma}_1 = \boldsymbol{B}_1\mathbf{\Lambda}_1\boldsymbol{B}_1' & \text{where} & \boldsymbol{B}_1 = [\boldsymbol{b}_1 \ldots \boldsymbol{b}_q : \boldsymbol{b}_{q+1(1)} \ldots \boldsymbol{b}_{p(1)}] \\ \mathbf{\Sigma}_2 = \boldsymbol{B}_2\mathbf{\Lambda}_2\boldsymbol{B}_2' & & \boldsymbol{B}_2 = [\boldsymbol{b}_1 \ldots \boldsymbol{b}_q : \boldsymbol{b}_{q+1(2)} \ldots \boldsymbol{b}_{p(2)}] \end{array}$$

Identifying the CPCs

Table 7.9. Decomposition of X^2_{total} in Head Dimension Example ($k = 2, p = 6$)

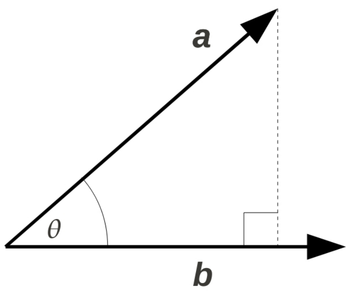
Model: Higher	Model: Lower	X^2	df	$\frac{X^2}{\text{df}}$	AIC for Higher Model
Equality	Proportionality	42.29	1	42.29	89.78
Proportionality	CPC	25.66	5	5.13	49.49
CPC	CPC(1)	15.12	10	1.51	33.82*
CPC(1)	Unrelated	6.70	5	1.34	38.70
Unrelated	---				42.0
Equality	Unrelated	89.78	21		

*Minimum AIC.

- χ^2 statistics not *independent*, and depend on *multivariate normality assumption*
- AIC not *formal hypothesis test*

Identifying the CPCs

Different approach (Krzanowski 1979)



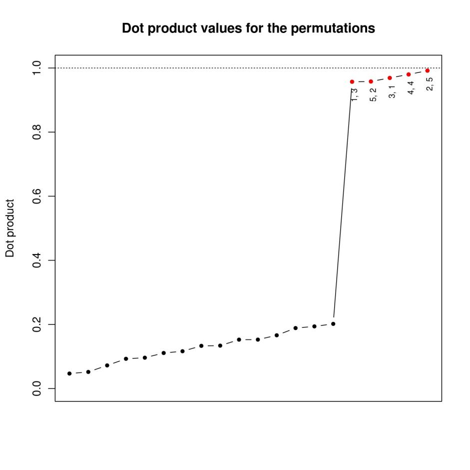
$\boldsymbol{a}'\boldsymbol{b} = \cos\theta$

- Inspect dot products from pairwise combinations of all p eigenvectors from the k groups

Identifying the CPCs

Simulated CPC data: $k = 2$, $p = 5$, $n = 200$

		Dot products
2	5	**0.99**
4	4	**0.98**
3	1	**0.97**
5	2	**0.96**
1	3	**0.96**
5	3	0.20
1	2	0.19
3	2	0.19
4	3	0.17
1	1	0.15



Identifying the CPCs

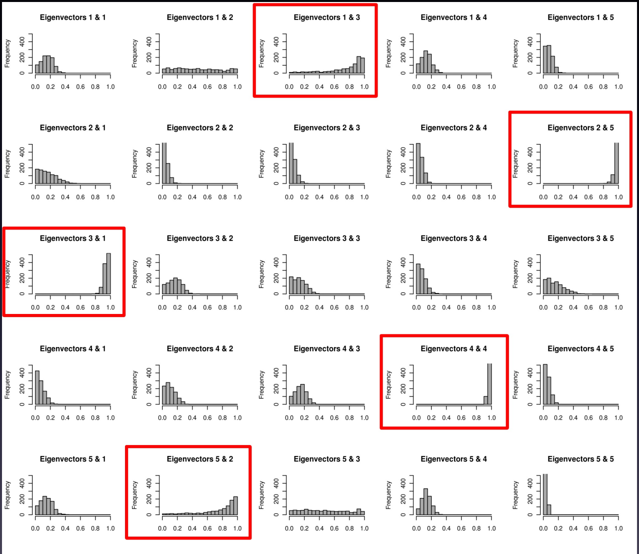
Simulated CPC data:

$k = 2$

$p = 5$

$n = 200$

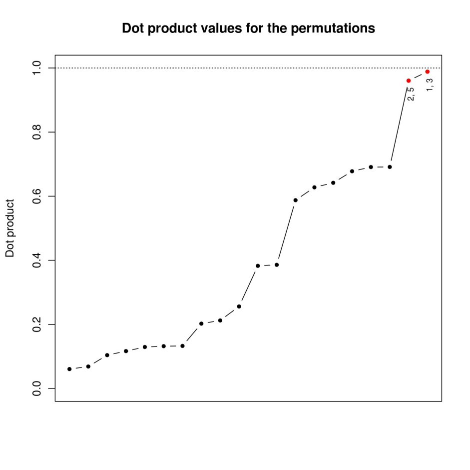
bootstrap reps $= 1000$



Identifying the CPCs

Simulated CPC(2) data: $k = 2$, $p = 5$, $n = 200$

		Dot products
1	3	**0.99**
2	5	**0.96**
3	4	0.69
4	2	0.69
5	2	0.68
3	1	0.64
5	1	0.63
4	4	0.59
4	1	0.39
5	4	0.38



Identifying the CPCs

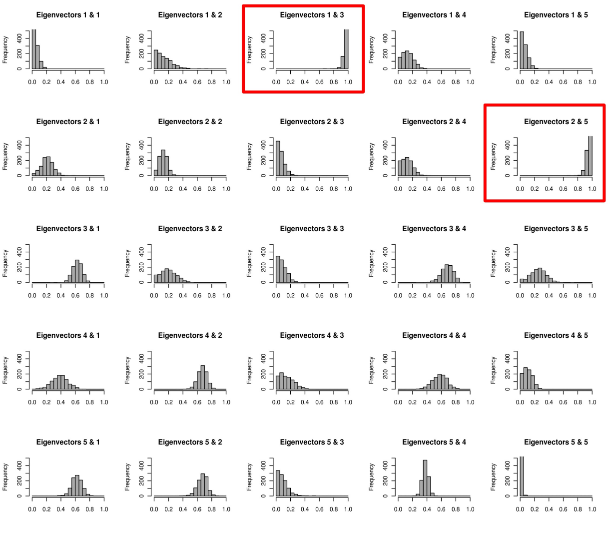
Simulated CPC(2) data:

$k = 2$

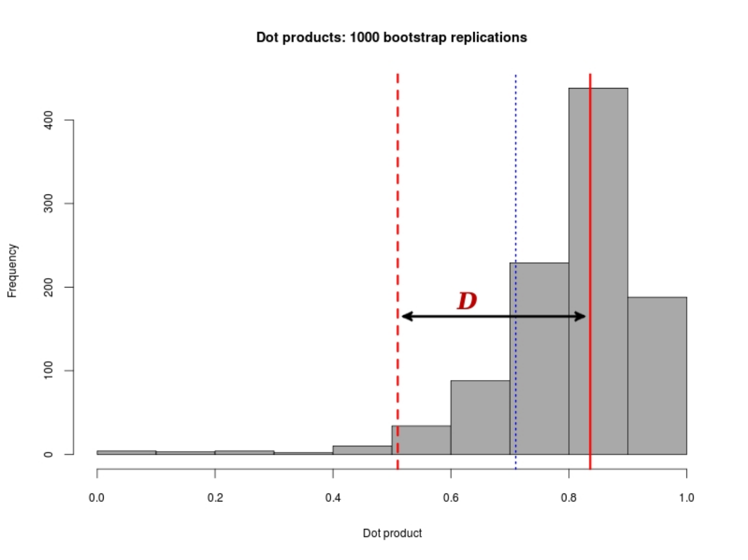
$p = 5$

$n = 200$

bootstrap reps $= 1000$



Identifying the CPCs



Identifying the CPCs

Bootstrap method:

1. Find median and 2.5^{th} percentile of bootstrap distribution
2. $D =$ median $- 2.5^{th}$ percentile
3. Then if
   - median > 0.71

     AND

   - median $+ D \geq 1$

   the two eigenvectors are deemed to be common

Simulation study

Simulation study

- Groups: $k = 2$
- Variables: $p = 5$
- Sample sizes: $n_i = 50, 100, 200, 500, 1000$
- Eigenvalues: poorly/moderately/well separated
- Normality: multivariate normal/non-normal
- Covariance structures: CPC, CPC(3), CPC(1), heterogeneity

Simulation study

Number of components correctly identified (%)

	AIC	χ^2	Bootstrap
Sample size			
$n = 50$	32	27	31
$n = 100$	41	29	36
$n = 200$	46	33	47
$n = 500$	50	32	61
$n = 1000$	50	35	74
Data			
Normal	50	34	54
Non-normal	38	28	46
Total	**44**	**31**	**50**

All methods fared slightly worse with non-normal data than with normal data.

Simulation study

Number of components correctly identified (%)

	AIC	χ^2	Bootstrap
Eigenvalue separation			
Poor (10%)	25	26	26
Moderate (50%)	49	32	53
Good (90%)	57	35	71
Covariance structure			
CPC	45	28	51
CPC(3)	34	20	28
CPC(1)	43	45	48
Heterogeneous	54	–	74
Total	**44**	**31**	**50**

Simulation study

Flury's AIC method:

- too greedy, especially for CPC(q)
- variability sometimes quite large
- best for small sample sizes
- performs well for full CPC with poorly separated eigenvalues

Simulation study

Flury's χ^2 method:

- poor performance overall
- large variability
- performed surprisingly well for CPC(1) with poorly separated eigenvalues

Simulation study

Bootstrap method:

- best for large sample sizes
- low variability
- does not perform well with poorly separated eigenvalues
- best for well separated eigenvalues, especially for non-normal data

Swiss heads data

Swiss heads data: $k = 2$, $p = 6$

Sample sizes: $n_1 = 200$, $n_2 = 59$

Eigenvalues:

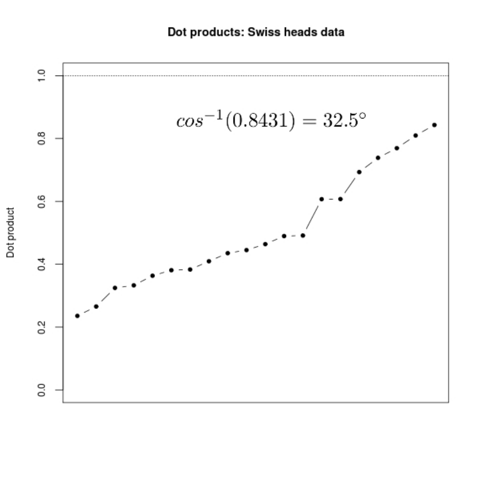
- Males: 66.3, 34.4, 19.6, 14.3, 13.0, 6.8
- Females: 73.5, 59.6, 42.0, 28.0, 15.6, 10.9
  (well separated in both groups)

Normality:

- Box's M test: $p < 0.0001$ (*not* multivariate normal)

Swiss heads data

		Dot products
5	6	0.84
6	5	0.81
2	3	0.77
1	2	0.74
3	4	0.69
4	4	0.61
1	1	0.61
2	2	0.49
3	1	0.49
4	1	0.46



Swiss heads data

Verdict on the number of common eigenvectors?

- Flury's AIC: 4
- Flury's χ^2: 3
- Bootstrap method: 0

Conclusions

- For smaller sample sizes and/or poorly separated eigenvalues
  $\rightarrow$ use Flury's AIC
- For larger sample sizes and well separated eigenvalues
  $\rightarrow$ use Bootstrap method
- Do not use Flury's χ^2 method

Sources

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- W. J. Krzanowski. *Between-groups comparison of principal components*. Journal of the American Statistical Association, 74(367): pp. 703-707, 1979.